Validation documentation
APIs & excipients, solid

HiperScan GmbH

March 7, 2025

Validation documentation of the chemometrics database of the near-infrared spectrometer *Apo-Ident*.
Report number: **50-2.9-2025-01**

Contents

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

Explanation of terminology 18

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

Validation reports 25
4-Aminobenzoic acid . . . 25
5-aminolevulinic acid hydrochloride . . . 29
Acacia, dried dispersion . . . 35
Acetylcysteine . . . 41
Acetylsalicylic acid . . . 47
Aciclovir . . . 55
Albendazole . . . 61
Alfatradiol . . . 67
Allantoin . . . 79
Allopurinol . . . 87
alpha-tocopheryl acetate dry concentrate . . . 93
Aluminium chloride hexahydrate . . . 99
Ambroxol hydrochloride . . . 107
Amifampridine . . . 119
Amiloride hydrochloride dihydrate . . . 125
Amitriptyline hydrochloride . . . 131
Amlodipine besilate . . . 139
Ammonium hydrogen carbonate . . . 143
Amoxicillin trihydrate . . . 149
Amphotericin B . . . 155
Arginine . . . 161
Arginine hydrochloride . . . 167
Ascorbic acid . . . 173
Ascorbyl palmitate . . . 181
Aspartic acid . . . 191
Atropine sulfate . . . 195
Bacitracin . . . 201
Baclofen . . . 209
Beclometasone dipropionate . . . 215
Benzocaine . . . 221
Benzoic acid . . . 231
Benzydamine hydrochloride . . . 237
Betaine monohydrate . . . 245
Betamethasone . . . 249
Betamethasone dipropionate . . . 255
Betamethasone valerate . . . 269
Bifonazole . . . 299
Biotin . . . 305
Bismuth gallath, basic . . . 311
Boric acid . . . 323

Budesonide . . . 329
Bupivacaine hydrochloride . . . 339
Butylated hydroxytoluene . . . 343
Caffeine . . . 351
Caffeine citrate . . . 359
Calcium ascorbate dihydrate . . . 365
Calcium citrate tetrahydrate . . . 371
Calcium gluconate . . . 379
Calcium glycerophosphate . . . 387
Calcium hydrogen phosphate dihydrate . . . 395
Calcium lactate pentahydrate . . . 401
Calcium pantothenate . . . 407
Camphor, racemic/D-Camphor . . . 415
Cannabidiol . . . 423
Capsaicin . . . 437
Captopril . . . 443
Carbomers . . . 453
Carmellose sodium . . . 465
Cellulose, microcrystalline . . . 473
Cetostearyl alcohol . . . 479
Chloral hydrate . . . 495
Chloramphenicol . . . 505
Chlorhexidine diacetate . . . 523
Chlorocresol . . . 533
Chlorprothixene hydrochloride . . . 539
Chlortetracycline hydrochloride . . . 543
Cholesterol . . . 553
Choline chloride . . . 561
Choline hydrogen tartrate . . . 565
Ciclopirox olamine . . . 571
Ciclosporin . . . 579
Ciprofloxacin hydrochloride . . . 587
Citric acid . . . 593
Citric acid monohydrate . . . 617
Citrulline . . . 625
Clindamycin hydrochloride . . . 631
Clindamycin-2-dihydrogen phosphate . . . 645
Clioquinol . . . 651
Clobetasol propionate . . . 667
Clonidine hydrochloride . . . 691
Clotrimazole . . . 697
Colistin sulfate . . . 731
Cyanocobalamin / Methylcobalamin . . . 737
Cyproheptadine hydrochloride 1.5 hydrate . . . 743
Cyproterone acetate . . . 747
Cysteine hydrochloride monohydrate . . . 755
Cystine . . . 761
Dequalinium chloride . . . 767
Dexamethasone . . . 777
Dexamethasone acetate . . . 795
Dextromethorphan hydrobromide monohydrate . . . 803
Diclofenac sodium . . . 809
Diltiazem hydrochloride . . . 819
Diphenhydramine hydrochloride . . . 843
Diphenylcyclopropenone . . . 849
Dithranol . . . 855
DL-Methionine . . . 865

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Doxepin hydrochloride . . . 869
Doxycycline hyclate . . . 875
Doxylamine hydrogen succinate . . . 881
EDTA calcium disodium . . . 887
Enalapril maleate . . . 893
Eosin Y . . . 899
Ephedrine hydrochloride . . . 905
Epinephrine hydrogen tartrate . . . 911
Erythromycin . . . 917
Escin, water-soluble . . . 951
Estradiol benzoate . . . 957
Estradiol hemihydrate . . . 967
Estradiol valerate . . . 977
Estriol . . . 987
Ethacridine lactate monohydrate . . . 997
Ethinylestradiol . . . 1005
Ethosuximide . . . 1011
Fampridine . . . 1015
Ferrous gluconate hydrate . . . 1021
Finasteride . . . 1025
Fluocinolone acetonide . . . 1031
Folic acid hydrate . . . 1037
Fructose . . . 1043
Furosemide . . . 1057
Fusidic acid . . . 1063
Gabapentin . . . 1069
Galactose . . . 1073
Gelatine, white . . . 1079
Gentamicin sulfate . . . 1085
Glucose . . . 1103
Glucose monohydrate . . . 1115
Glutamic acid . . . 1137
Glutamine . . . 1143
Glutathione . . . 1149
Glycine . . . 1155
Glycopyrronium bromide . . . 1161
Gramicidin . . . 1167
Griseofulvin . . . 1173
Guaifenesin . . . 1179
Heparin sodium . . . 1185
Histamine dihydrochloride . . . 1191
Histidine . . . 1197
Homatropine hydrobromide . . . 1203
Hydrochlorothiazide . . . 1207
Hydrocortisone . . . 1215
Hydrocortisone acetate . . . 1239
Hydroquinone . . . 1265
Hydroxyethyl cellulose . . . 1273
Hyoscine butylbromide . . . 1279
Hyoscine hydrobromide . . . 1285
Ibuprofen . . . 1293
Indometacin . . . 1299
Iodoform . . . 1305
Ipratropium bromide . . . 1315
Isoleucine . . . 1321
Isosorbide dinitrate 40% . . . 1327
Isoxsuprine hydrochloride . . . 1339

Ivermectin 1343
Ketamine hydrochloride 1347
Ketoconazole 1353
Lactose monohydrate 1359
L-alanine 1377
Leucine 1381
Levocarnitine 1387
Levothyroxin sodium 1393
Lidocaine 1399
Lidocaine hydrochloride monohydrate 1415
Lithium orotate monohydrate 1435
L-Phenylalanine 1441
L-Threonine 1447
Lysine hydrochloride 1453
Macrogols 1500 1459
Macrogols 4000 1465
Mafenide acetate 1485
Magnesium chloride hexahydrate 1489
Magnesium citrate 1495
Magnesium hydrogen aspartate tetrahydrate 1501
Magnesium hydrogen citrate 1507
Magnesium orotate dihydrate 1519
Magnesium stearate 1525
Magnesium sulfate heptahydrate 1531
Maltodextrin 1537
Manganese orotate dihydrate 1543
Manganese sulfate monohydrate 1549
Mannitol 1553
Melatonin 1579
Menthol 1593
Mepivacaine hydrochloride 1611
Mesalazine 1617
Metamizol sodium monohydrate 1623
Methacholine chloride 1629
Methionine 1635
Methoxsalen 1641
Methyl-4-hydroxybenzoate 1651
Methylcellulose 1659
Methylprednisolone 1671
Metoclopramide hydrochloride monohydrate 1677
Metoprolol tartrate 1683
Metronidazole 1689
Miconazole nitrate 1717
Minoxidil 1737
Mometasone furoate 1759
Monostereates 1779
Mupirocin calcium 1789
myo-Inositol 1795
Naloxone hydrochloride dihydrate 1799
Naltrexone hydrochloride 1805
Naphazoline hydrochloride 1809
Naphazoline nitrate 1817
Naproxen 1823
Neomycin sulfate 1827
Neostigmine bromide 1839
Nicotinamide 1845
Nicotinic acid 1851

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Nifedipine 1857
Nitrofurantoin 1861
Non-ionic emulsifying alcohol 1867
Norethisterone acetate 1873
Noscapine hydrochloride hydrate 1879
Nystatin 1883
Octenidine dihydrochloride 1899
Ofloxacin 1913
Omeprazole 1919
Ornithine aspartate 1927
Ornithine hydrochloride 1933
Oxalic acid 1939
Oxetacaine 1945
Oxybuprocaine hydrochloride 1951
Oxybutynin hydrochloride 1957
Oxytetracycline hydrochloride 1965
Pancreas powder 1975
Papaverine hydrochloride 1979
Paracetamol 1985
Patent blue V 1993
Pectin 1999
Phenazone 2003
Pheniramine maleate 2009
Phenylbutazon 2015
Phenylephrine hydrochloride 2021
Phenytoin 2027
Pilocarpine hydrochloride 2033
Poloxamers 2039
Polymyxin B sulfate 2045
Potassium citrate 2053
potassium dihydrogen phosphate 2063
Potassium hydrocarbonate 2067
Potassium hydrogen tartrate 2073
Potassium sorbate 2079
Povidone 2093
Povidone iodine 2101
Prasterone 2109
Praziquantel 2117
Prednicarbate 2121
Prednisolon dihydrogen phosphate dinatrium 2143
Prednisolone 2151
Prednisolone acetate 2171
Prednisolone hydrogen succinate 2191
Prednisone 2197
Pregnenolone 2203
Prilocaine 2209
Prilocaine hydrochloride 2213
Procaine hydrochloride 2219
Progesterone 2227
Proline 2247
Propranolol hydrochloride 2253
Propyl-4-hydroxybenzoate 2265
Propyphenazone 2271
Pyridoxal-5-phosphate 2277
Pyridoxine hydrochloride 2283
Quetiapine fumarate 2289
Quinidine sulfate dihydrate 2293

Quinine hydrochloride dihydrate 2299
Quinine sulfate 2305
Quinoline yellow 2311
Resocrinol 2317
Riboflavin 2325
Riboflavin sodium phosphate hydrate 2333
Ropivacaine hydrochloride monohydrate 2339
Saccharin sodium 2343
Salbutamol sulfate 2351
Salicylic acid 2355
Selenium yeast 2379
Serine 2385
Sildenafil citrate 2391
Silver protein 2401
Sodium acetate trihydrate 2407
Sodium ascorbate 2413
Sodium benzoate 2419
Sodium chondroitin sulfate 2429
Sodium citrate 2433
Sodium cromoglicate 2451
Sodium cyclamate 2457
Sodium dihydrogen phosphate dihydrate 2463
Sodium edetate 2469
Sodium salicylate 2481
Sodium sulfate decahydrate 2487
Sodium tetraborate 2493
Sorbic acid 2499
Sorbitol 2507
Sotalol hydrochloride 2515
Soy lecithin (instant form) 2519
Spironolactone 2525
Starch 2537
Stearic acid 50 2555
Sucrose 2561
Sulfacetamide 2581
Sulfadiazine 2587
Sulfogaiacol hydrate 2593
Sulpiride 2599
Tacrolimus monohydrate 2603
Tannin 2609
Tartaric acid 2619
Taurine 2629
Testosterone 2635
Testosterone propionate 2643
Tetracaine 2655
Tetracaine hydrochloride 2665
Tetracycline hydrochloride 2681
Theophylline 2691
Theophylline-ethylenediamine hydrate 2697
Thiamine chloride hydrochloride 2703
Thiomersal 2709
Thymol 2715
Tobramycin sulfate 2723
Tosylchloramide sodium 2729
Tranexamic acid 2735
Tretinoin 2741
Triamcinolone 2757

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Triamcinolone acetonide 2763
Triclosan 2793
Trometamol 2823
Tropicamide 2835
Tryptophan 2841
Tyrosine 2847
Tyrothricin 2853
Ubidecarenone 2859
Urea 2865
Ursodeoxycholic acid 2893
Valine 2897
Vancomycin hydrochloride 2903
Vanillin 2909
Waxes / Fats 2915
Wool alcohols 2951
Xylitol 2957
Xylometazoline hydrochloride 2963
Xylose 2971
Zinc acetate dihydrate 2977
Zinc gluconate 2983
Zinc orotate dihydrate 2989
Zinc stearate 2993
Zinc sulfate heptahydrate 2997

Appendix **3003**
Additional calibration samples (*Type A*) 3003
Additional validation samples (*Type B*) 3009
Additional validation samples (*Type C*) 3035
Requirements of validation 3171
Conformity of *Apo-Ident* with the *European pharmacopeia* 3172
Addition to the second-stage models 3173

References **3177**

Index **3179**

Introduction

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

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

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

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

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

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

Context of this document

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

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

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

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

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

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

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

Criteria for the inclusion of substances

This validation documentation describes the results of the validation of the reference database for the substance class *APIs & excipients, solid*. Validation documentation is created for each published version of the reference database for all substance classes incorporated.

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

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

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

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

Validation concept

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

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

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

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

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

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

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

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

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

Model creation procedure and validation runs

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

1. Collecting the reference spectra (calibration sample)

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

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

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

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

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

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

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

2. Generating the chemometric models (calibration)

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

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

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

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

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

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

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

3. Set of validation spectra (validation samples)

The following is provided for validation:

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

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

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

All manufacturers' batches from which spectra are used for the validation are listed by substance in this document: for substances included in the substance class *APIs & excipients, solid* in the respective validation reports; otherwise in attachments *A*, *B* and *C*.

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

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

4. Validation runs and approval

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

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

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

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

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

Particularities of individual substance classes

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

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

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

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

Significance of testing with *Apo-Ident*

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

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

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

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

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

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

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

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

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

Conclusion

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

Explanation of terminology

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

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

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

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

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

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

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

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

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

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

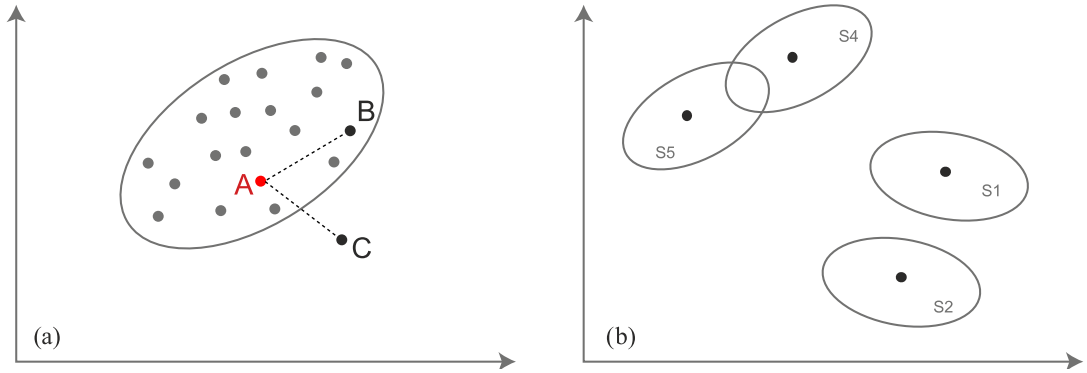


Figure 1: (a) The *Mahalanobis distance* from A to B is less than from A to C. However, the Euclidean distances are identical. (b) The *Mahalanobis distance* between the two measurement series *S4* and *S5* is smaller than between *S1* and *S2*. However, the Euclidean distances are identical.

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

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

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

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

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

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

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

Summary

A total of 591 113 spectra from 54 984 different batches for a total of 953 substances were used to validate the substance class *APIs & excipients, solid*.

Validation samples

The validation samples can be categorised as follows:

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

Substance class	Substances	Batches	Spectra
APIs & excipients, solid	394	2663	141 912
APIs & excipients, solid (BR)	10	15	640
Specific classifier 26188	17	37	1750
Narcotic substances, solid	13	66	6000
Drugs	52	61	2660

From category *A* a total of 152 962 spectra from 2842 batches for a total of 486 substances were taken into account for validation.

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

Substance class	Substances	Batches	Spectra
APIs & excipients, solid	530	3333	167 782
APIs & excipients, solid (BR)	27	46	2220
Drugs	250	575	25 703
Specific classifier 26188	12	23	1019
Narcotic substances, solid	17	66	5040
Chemicals, solid	8	8	320

From category *B* a total of 202 084 spectra from 4051 batches for a total of 844 substances were taken into account for validation.

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

Substance class	Substances	Batches	Spectra
APIs & excipients, solid	418	43 125	219 225
Drugs	286	6038	14 406
Narcotic substances, solid	15	894	2428
Specific classifier 26188	3	7	8

From category *C* a total of 236 067 spectra from 50 064 batches for a total of 722 substances were taken into account for validation.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	140 629	53	53 090 094
Type B	0	151 854	219	70 172 885
Type C	0	214 305	2715	81 933 513

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

	Specificity	Recognition rate
Type A	100.000 00 % (> 99.999 97 %)	99.976 30 % (> 99.973 37 %)
Type B	100.000 00 % (> 99.999 97 %)	99.683 53 % (> 99.678 96 %)
Type C	100.000 00 % (> 99.999 71 %)	98.440 63 % (> 98.379 85 %)

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

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**4-Aminobenzoic acid**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10005947-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

4-Aminobenzoic acid; Acidum 4-aminobenzoicum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
4-Aminobenzoic acid	4	1	0

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Oxytetracycline hydrochloride	177.78	–

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

Calibration samples

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

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

Validation samples

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

Type A All calibration spectra.

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

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 772 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

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

- 202 004 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

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

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

Validation results

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

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

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

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25867	25867	0.00	297.23
26050	26050	0.00	297.98
26207	26207	0.00	298.54
26754	26754	0.00	297.75

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**5-aminolevulinic acid hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20371-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

5-aminolevulinic acid hydrochloride; Acidum aminolaevulinicum hydrochloricum

Special notes

When selecting the *5-aminolevulinic acid hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
5-aminolevulinic acid hydrochloride	7	6	83

Second-stage model

For differentiation of the substance/substance group *5-aminolevulinic acid hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *5-aminolevulinic acid hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Menthol	100.80	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *5-aminolevulinic acid hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *5-aminolevulinic acid hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	5-aminolevulinic acid hyd…	16357904	23208	40	1707616
Caelo	5-aminolevulinic acid hyd…	16357904	23747	40	20170324
Caelo	5-aminolevulinic acid hyd…	190219	24733	40	20190312*
Caelo	5-aminolevulinic acid hyd…	192811002	25371	40	20191107
Caelo	5-aminolevulinic acid hyd…	20004269	25645	40	20210202*
Fagron	5-aminolevulinic acid hyd…	13K27-N02	21339	40	20131125
Fagron	5-aminolevulinic acid hyd…	17A12-B07-332960	23403	40	20170131
Fagron	5-aminolevulinic acid hyd…	17A12-B07-332960	23404	40	20170131
Fagron	5-aminolevulinic acid hyd…	19K14-F02-366541	25372	40	20191209

Validation samples

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

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *5-aminolevulinic acid hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 602 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 335 spectra of 11 reference samples from the substance/substance group *5-aminolevulinic acid hydrochloride*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	5-aminolevulinic acid hyd…	22003347	26505	40
Fagron	5-aminolevulinic acid hyd…	18C16-B05-347714	24099	40
Fagron	5-aminolevulinic acid hyd…	21G28-B05-216542	25843	50
Fagron	5-aminolevulinic acid hyd…	21L14-B01-220727	26082	40
Fagron	5-aminolevulinic acid hyd…	22B16-B03-218068	26297	40
Fagron	5-aminolevulinic acid hyd…	23B17-B04-227315	26685	40
Caelo	5-aminolevulinic acid hyd…	22003347	26505SI	20
Fagron	5-aminolevulinic acid hyd…	21G28-B05-216542	25843SI	15
Fagron	5-aminolevulinic acid hyd…	21L14-B01-220727	26082SI	10
Fagron	5-aminolevulinic acid hyd…	22B16-B03-218068	26297SI	20
Fagron	5-aminolevulinic acid hyd…	23B17-B04-227315	26685SI	20

- 201 749 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 116 spectra from 42 *Apo-Ident* customers from 87 batches from the substance/substance group *5-aminolevulinic acid hydrochloride*.

- Among them are spectra of independent samples from 83 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	5-aminolevulinic acid hyd…	13C-19-N07	1
	5-aminolevulinic acid hyd…	23B17-B04-227317	1
Biosynth AG / Otto	5-aminolevulinic acid hyd…	20563	1
Biosynth AG	5-aminolevulinic acid hyd…	F05-3695208	1
Caelo	5-aminolevulinic acid hyd…	11355616	1
Caelo	5-aminolevulinic acid hyd…	12093205	2
Caelo	5-aminolevulinic acid hyd…	12093208	1
Caelo	5-aminolevulinic acid hyd…	13017402	1
Caelo	5-aminolevulinic acid hyd…	13017403	1
Caelo	5-aminolevulinic acid hyd…	13K27-N02	1
Caelo	5-aminolevulinic acid hyd…	14145003	2
Caelo	5-aminolevulinic acid hyd…	14145007	3
Caelo	5-aminolevulinic acid hyd…	14145011	1
Caelo	5-aminolevulinic acid hyd…	15254803	1
Caelo	5-aminolevulinic acid hyd…	16357902	1
Caelo	5-aminolevulinic acid hyd…	16357910	1
Caelo	5-aminolevulinic acid hyd…	18026102	1
Caelo	5-aminolevulinic acid hyd…	18C16-B05-347711	1
Caelo	5-aminolevulinic acid hyd…	18C16-B05-37711	1
Caelo	5-aminolevulinic acid hyd…	19281105	1
Caeolo	5-aminolevulinic acid hyd…	15254803	1
Caesar & Loretz GmbH	5-aminolevulinic acid hyd…	192811002	1
Caesar & Loretz GmbH	5-aminolevulinic acid hyd…	20004269005	1
Caesar & Loretz GmbH	5-aminolevulinic acid hyd…	22003347002	1
Euro OTC	5-aminolevulinic acid hyd…	18L03-B01-357231	1
Fagron	5-aminolevulinic acid hyd…	11I30-N01	1
Fagron	5-aminolevulinic acid hyd…	12c23-n05	1
Fagron	5-aminolevulinic acid hyd…	12H20-N01	1
Fagron	5-aminolevulinic acid hyd…	12K26-N05	1
Fagron	5-aminolevulinic acid hyd…	13C19-N05	3
Fagron	5-aminolevulinic acid hyd…	13G18-B06-355728	1
Fagron	5-aminolevulinic acid hyd…	13H13-N07	2
Fagron	5-aminolevulinic acid hyd…	13J29-N03	2
Fagron	5-aminolevulinic acid hyd…	13K27-N02	2
Fagron	5-aminolevulinic acid hyd…	14802	1
Fagron	5-aminolevulinic acid hyd…	14K04-B01-297971	2
Fagron	5-aminolevulinic acid hyd…	14K13-B01	1
Fagron	5-aminolevulinic acid hyd…	15C06-B02-305245	1
Fagron	5-aminolevulinic acid hyd…	15J23-B06	1
Fagron	5-aminolevulinic acid hyd…	15J23-B06-314284	1
Fagron	5-aminolevulinic acid hyd…	16A11-B02	1
Fagron	5-aminolevulinic acid hyd…	16A11-B02-316734	1
Fagron	5-aminolevulinic acid hyd…	16A11-B02-317459	3
Fagron	5-aminolevulinic acid hyd…	16A11-B02-318406	1
Fagron	5-aminolevulinic acid hyd…	16E17-B08-324962	2
Fagron	5-aminolevulinic acid hyd…	16G27-B10	1
Fagron	5-aminolevulinic acid hyd…	16I12-B06	1
Fagron	5-aminolevulinic acid hyd…	16I12-B06-326185	1
Fagron	5-aminolevulinic acid hyd…	16K17-B09-328197	1
Fagron	5-aminolevulinic acid hyd…	16K17-B09-330371	1
Fagron	5-aminolevulinic acid hyd…	17/22-B02-342555	1
Fagron	5-aminolevulinic acid hyd…	1701-b05-342090	1
Fagron	5-aminolevulinic acid hyd…	17A12-B07-331744	1
Fagron	5-aminolevulinic acid hyd…	17A12-B07-331745	1
Fagron	5-aminolevulinic acid hyd…	17F01-B05-338204	1
Fagron	5-aminolevulinic acid hyd…	17F01-B06_337165	1
Fagron	5-aminolevulinic acid hyd…	17F01-B06-337163	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	5-aminolevulinic acid hyd…	17F01-B06-337164	2
Fagron	5-aminolevulinic acid hyd…	17I22-B02	3
Fagron	5-aminolevulinic acid hyd…	17I22-B02-343410	1
Fagron	5-aminolevulinic acid hyd…	17I22-B02-343411	1
Fagron	5-aminolevulinic acid hyd…	17L18-B05-344673	1
Fagron	5-aminolevulinic acid hyd…	17l22-B02-343410	1
Fagron	5-aminolevulinic acid hyd…	18C16-B05	4
Fagron	5-aminolevulinic acid hyd…	18C16-B05-347714	1
Fagron	5-aminolevulinic acid hyd…	18D10-B02-361711	1
Fagron	5-aminolevulinic acid hyd…	18D17-B02349681	1
Fagron	5-aminolevulinic acid hyd…	18G13-806-352897	1
Fagron	5-aminolevulinic acid hyd…	18G13-B06	2
Fagron	5-aminolevulinic acid hyd…	18G13-B06-355728	1
Fagron	5-aminolevulinic acid hyd…	18L03-B01	1
Fagron	5-aminolevulinic acid hyd…	18L03-B01-360101	1
Fagron	5-aminolevulinic acid hyd…	19G31-B02	5
Fagron	5-aminolevulinic acid hyd…	19G31-B02-363475	1
Fagron	5-aminolevulinic acid hyd…	19G31-B02-364671	1
Fagron	5-aminolevulinic acid hyd…	19G31-B02-364672	1
Fagron	5-aminolevulinic acid hyd…	19G31-B02-36473	1
Fagron	5-aminolevulinic acid hyd…	19K14-F02-366541	1
Fagron	5-aminolevulinic acid hyd…	19K14-F02-366544	1
Fagron	5-aminolevulinic acid hyd…	19K14-F02-368326	1
Fagron	5-aminolevulinic acid hyd…	20A29-F05-367867	1
Fagron	5-aminolevulinic acid hyd…	20A29-F05-369528	1
Fagron	5-aminolevulinic acid hyd…	20F04-F01-371115	1
Fagron	5-aminolevulinic acid hyd…	20F04-F02-371121	1
Fagron	5-aminolevulinic acid hyd…	21G28-B05-213714	2
Fagron	5-aminolevulinic acid hyd…	22H03-B02-225921	1
Fagron	5-aminolevulinic acid hyd…	23B17-B04-227317	1
Fagron	5-aminolevulinic acid hyd…	25414	1
Fagron	5-aminolevulinic acid hyd…	7447	1
Fiebig	5-aminolevulinic acid hyd…	18c16-b05-347711	1

- 235 951 spectra from 1515 *Apo-Ident* customers from a total of 49 172 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *5-aminolevulinic acid hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *5-aminolevulinic acid hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	335	0	201 749
Type C	0	114	2	235 951

The substance/substance group *5-aminolevulinic acid hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.2090 %)
Type C	100.0000 % (> 99.9007 %)	98.2759 % (> 95.6897 %)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21339	23208	55.78	127.69
23208	23208	0.00	127.97
23403	23208	47.00	126.23
23404	23208	39.21	127.16
23747	23208	6.01	127.92
24733	24733	0.00	123.82
25371	23208	37.98	129.79
25372	23208	45.59	126.98
25645	25645	0.00	127.15

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Acacia, dried dispersion**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20457-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Acacia, dried dispersion; Acaciae gummi dispersione desiccatum

Special notes

When selecting the *Acacia, dried dispersion* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Acacia, dried dispersion	6	3	13

Second-stage model

For differentiation of the substance/substance group *Acacia, dried dispersion* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
SyrSpend® SF pH4	31.08	14.74
SyrSpend® SF Alka	36.52	24.69
Rice starch	42.29	25.18
SyrSpend® SF pH4 neo (Maize starch)	43.81	16.10
Wheat starch	52.59	21.57
⋮	⋮	⋮
Carmellose sodium	>50	23.78
Corn starch	>50	26.09
Colistin sulfate	>50	29.02
Polymyxin B sulfate	>50	32.08
Maltodextrin	>50	32.18
Calcium glycerophosphate	>50	32.56
Potato starch	>50	33.46
Amphotericin B	>50	45.81
Cyanocobalamin	>50	48.78
Bacitracin	>50	52.95
Riboflavin	>50	60.82
Selenium yeast	>50	68.14
Tosylchloramide sodium	>50	81.31
Calcium pantothenate	>50	84.12
Nystatin	>50	85.74
Oxalic acid	>50	92.52
Fructose	>50	97.16
Gelatine, white	>50	102.27
Hyoscine hydrobromide	>50	108.17
Estradiol hemihydrate	>50	132.23
Triamcinolone	>50	132.79
alpha-tocopheryl acetate dry concentrate	>50	133.00
Estriol	>50	169.90
Methylcobalamin	>50	173.29

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Acacia, dried dispersion	14141901	21431	120	AR-15-FG-006809-01
Caelo	Acacia, dried dispersion	15413201	22653	40	AR-17-FG-000844-01
Caelo	Acacia, dried dispersion	181860	24730	40	20180725*
Caelo	Acacia, dried dispersion	192248013	25501	40	20190828
Caelo	Acacia, dried dispersion	24001100	27261	40	20240604*
Caelo	Acacia, dried dispersion	24002524	27443	40	20241105*

Validation samples

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

Type A All calibration spectra.

- 320 spectra of 6 reference samples from the substance/substance group *Acacia, dried dispersion*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 210 spectra of 7 reference samples from the substance/substance group *Acacia, dried dispersion*.

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

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Acacia, dried dispersion	162331	22853	40
Caelo	Acacia, dried dispersion	16233105	23443	40
Caelo	Acacia, dried dispersion	21003060	25982	40

continued on the next page

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

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Acacia, dried dispersion	16233105	23444	40
Caelo	Acacia, dried dispersion	21003060	25982SI	10
Caelo	Acacia, dried dispersion	24001100	27261SI†	20
Caelo	Acacia, dried dispersion	24002524	27443SI†	20

- 201 874 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 15 spectra from 13 *Apo-Ident* customers from 14 batches from the substance/substance group *Acacia, dried dispersion*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Acacia, dried dispersion	11345715	1
Caelo	Acacia, dried dispersion	12111301	1
Caelo	Acacia, dried dispersion	12138607	1
Caelo	Acacia, dried dispersion	12138612	1
Caelo	Acacia, dried dispersion	12372302	1
Caelo	Acacia, dried dispersion	15086704	1
Caelo	Acacia, dried dispersion	15413201	1
Caelo	Acacia, dried dispersion	15413207	1
Caelo	Acacia, dried dispersion	16233105	2
Caelo	Acacia, dried dispersion	21003060011	1
Caelo	Acacia, dried dispersion	3314A160121	1
Caesar & Loretz GmbH	Acacia, dried dispersion	18186001	1
Klenk	Acacia, dried dispersion	3314A140121	1
ROHA	Acacia, dried dispersion	170190	1

- 236 052 spectra from 1515 *Apo-Ident* customers from a total of 49 244 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Acacia, dried dispersion* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Acacia, dried dispersion* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect.

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	210	0	201 874
Type C	0	15	0	236 052

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.1429 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21431	21431	0.00	41.92
22653	22653	0.00	36.02
24730	24730	0.00	39.77
25501	22653	6.70	38.18
27261	27261	0.00	35.33
27443	27443	0.00	37.13

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

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Acetylcysteine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20040-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Acetylcysteine; Acetylcysteinum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

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

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	116.28	–

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

Calibration samples

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

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

Validation samples

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

Type A All calibration spectra.

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

- 152 622 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

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

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

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

- 201 394 spectra from a total of 4029 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

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

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

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

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

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

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

Validation results

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

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

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

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21315	22228	15.34	213.83
21628	22469	12.38	196.88
22228	22228	0.00	214.73
22469	22469	0.00	199.19
22854	22854	0.00	215.45
22886	22228	13.62	216.96
26090	26090	0.00	226.73

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Acetylsalicylic acid**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20449-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Acetylsalicylic acid; Acidum acetylsalicylicum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Acetylsalicylic acid	7	9	102

Second-stage model

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

- Submodel 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Midazolam hydrochloride	87.74	–
⋮	⋮	⋮
Dithranol	>50	17.02
Dequalinium chloride	>50	52.48
Sodium salicylate	>50	69.40
Benzoic acid	>50	79.93
Eosin Y	>50	252.87
Oxytetracycline hydrochloride	>50	357.71
Levothyroxin sodium	>50	683.56
Tannin	>50	1569.01

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

Calibration samples

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

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

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

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

Type A All calibration spectra.

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

- 152 657 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 400 spectra of 12 reference samples from the substance/substance group *Acetylsalicylic acid*.

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

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

- 201 684 spectra from a total of 4036 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

descend.

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

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

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

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

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

continued on the next page

continued from previous page

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

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

Validation results

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

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

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

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21383	22377	12.42	117.23
21597	22377	13.56	115.96
21637	22377	22.01	118.28
22377	22377	0.00	117.88
22820	22820	0.00	116.54
22949	22377	10.74	115.01
23064	23064	0.00	116.71

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

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Aciclovir**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21677-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Aciclovir; Aciclovirum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

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

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	86.41	–

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

Calibration samples

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

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

Validation samples

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

Type A All calibration spectra.

- 290 spectra of 6 reference samples from the substance/substance group *Aciclovir*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.
- 152 672 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

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

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

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

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

- 201 864 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

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

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

continued on the next page

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

continued from previous page

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

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

Validation results

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

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

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

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

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21677	21677	0.00	204.64
21761	21677	7.32	203.16
21831	21677	17.73	204.68
25064	21677	14.62	200.89
27099	21677	14.49	204.52
27381	21677	8.58	200.89

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

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Albendazole**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21596-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Albendazole; Albendazolum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Albendazole	6	3	14

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Clonidine hydrochloride	165.58	–

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Albendazole	2208010	26263	40	20220831*
Euro OTC	Albendazole	2208010	26263SI	20	20220831*
Fagron	Albendazole	12J25-B40-293217	21596	45	AR-15-FG-002571-01
Fagron	Albendazole	16B04-B06-329519	23017	40	20160302
Fagron	Albendazole	18C21-B04-351586	24578	40	20180625
Fagron	Albendazole	20B27-F01-373154	25714	40	20200901
Fagron	Albendazole	22B26-B05-219216	26174	40	20220602

Validation samples

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

Type A All calibration spectra.

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 265 spectra of 7 reference samples from the substance/substance group *Albendazole*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 697 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 160 spectra of 4 reference samples from the substance/substance group *Albendazole*.

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

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Albendazole	14B05-B41-299704	21730	60
Fagron	Albendazole	14B05-B41-314321	22940	40
Fagron	Albendazole	16B04-B06-322057	22968	40
Fagron	Albendazole	22B26-B05-219216	26174SI†	20

- 201 924 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 28 spectra from 14 *Apo-Ident* customers from 17 batches from the substance/substance group *Albendazole*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

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

Supplier	Substance	Batch	Spectra
Fagron	Albendazole	14B05-B41	1
Fagron	Albendazole	14B05-B41-305249	1
Fagron	Albendazole	14B05B41-312959	1
Fagron	Albendazole	14B05-B41-312959	1
Fagron	Albendazole	14b05-b41-314321	1
Fagron	Albendazole	14B05-B41-314321	1
Fagron	Albendazole	16B04-B06-322055	2
Fagron	Albendazole	16B04-B06-329519	1
Fagron	Albendazole	16B04-B06-337998	2
Fagron	Albendazole	18C21-B04	1
Fagron	Albendazole	18C21-B04-350057	1
Fagron	Albendazole	18C21-B04-351584	1
Fagron	Albendazole	18C21-B04-351585	3
Fagron	Albendazole	18C21-B04-351586	4
Fagron	Albendazole	18C21-B04-357034	1
Fagron	Albendazole	18C21-B04x3	1
Fagron	Albendazole	20B27-F01-373151	5

- 236 039 spectra from 1515 *Apo-Ident* customers from a total of 49 241 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	265	0	152 697
Type B	0	160	0	201 924
Type C	0	28	0	236 039

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7358 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 78.5714 %)

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

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21596	21596	0.00	287.83
23017	26263	16.75	296.36
24578	26263	13.40	306.22
25714	26263	12.33	302.73
26174	26263	9.13	302.86
26263	26263	0.00	303.66

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

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Alfatradiol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20292-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Alfatradiol; Alfatradiolum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Alfatradiol	10	18	262

Second-stage model

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

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	82.13	–
⋮	⋮	⋮
Capsaicin	>50	58.00
Levocarnitine	>50	120.77
Prednicarbate	>50	136.43
Sodium citrate	>50	139.94
Oxybutynin hydrochloride	>50	152.64
Pyridoxal-5-phosphate	>50	203.70
Norethisterone acetate	>50	208.68
Tetracaine	>50	217.64
Cyproterone acetate	>50	261.51
Amitriptyline hydrochloride	>50	449.51
Quinine hydrochloride dihydrate	>50	470.77
Methoxsalen	>50	574.96
Heparin sodium	>50	604.20
Valine	>50	650.36
Ciprofloxacin hydrochloride	>50	771.14
Amifampridine	>50	1497.50
Triclosan	>50	1598.25
Sucrose	>50	1997.63

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Alfatradiol	AP33-16-I-62P2985A	22935	40	20161017
Audor Pharma	Alfatradiol	AP33-18-I-68P3620A	24662	40	20180804

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Alfatradiol	13201601	21476	120	20130812
Caelo	Alfatradiol	13201601	21477	60	20130812
Caelo	Alfatradiol	191599	24747	40	20190812*
Caelo	Alfatradiol	20004170	25553	40	20210106*
Caelo	Alfatradiol	20004170	25553SI	40	20210106*
Caelo	Alfatradiol	20002390	25561	40	20200914*
Caelo	Alfatradiol	20002390	25561SI	40	20200914*
Euro OTC	Alfatradiol	1404001-01	21714	50	1509288
Euro OTC	Alfatradiol	1404001-01	21714SI	60	1509288
Euro OTC	Alfatradiol	1603019	22511	40	20160419*
Euro OTC	Alfatradiol	1603019	22511SI	40	20160419*
Fagron	Alfatradiol	13G19-N06	20940	40	1402683
Fagron	Alfatradiol	15J27-B08-323877	22933	40	20151117
Fagron	Alfatradiol	15J27-B08-323877	22934	40	20151117
Fagron	Alfatradiol	15J27-B08-323877	22934SI	40	20151117

Validation samples

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

Type A All calibration spectra.

- 810 spectra of 17 reference samples from the substance/substance group *Alfatradiol*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 152 spectra from a total of 2832 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 1654 spectra of 41 reference samples from the substance/substance group *Alfatradiol*.

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

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

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Alfatradiol	161804	23354	40
Caelo	Alfatradiol	191598	24738	40
Caelo	Alfatradiol	22000052006	26740	40
Euro OTC	Alfatradiol	1902020	24621	40
Euro OTC	Alfatradiol	2002017	25118	40
Euro OTC	Alfatradiol	2006005	25473	40
Euro OTC	Alfatradiol	2103003	25689	50
Euro OTC	Alfatradiol	2201003	25948	40
Euro OTC	Alfatradiol	2301040	26601	40
Euro OTC	Alfatradiol	2305010	26755	40
Euro OTC	Alfatradiol	2305011	26756	30
Euro OTC	Alfatradiol	2305012	26757	30
Euro OTC	Alfatradiol	2305013	26758	40
Euro OTC	Alfatradiol	2305014	26759	40
Euro OTC	Alfatradiol	2310012	26998	40
Euro OTC	Alfatradiol	2409001	27388	40
Euro OTC	Alfatradiol	2409008	27389	40
Fagron	Alfatradiol	22I06-B02-222372	26390	40
Audor Pharma	Alfatradiol	AP33-16-I-62P2985A	22935SI[†]	40
Audor Pharma	Alfatradiol	AP33-18-I-68P3620A	24662SI[†]	40
Caelo	Alfatradiol	13201601	21477SI[†]	60
Caelo	Alfatradiol	161804	23354SI	40
Caelo	Alfatradiol	191598	24738SI	40
Caelo	Alfatradiol	191599	24747SI[†]	40
Caelo	Alfatradiol	22000052006	26740SI	40
Euro OTC	Alfatradiol	1902020	24621SI	40
Euro OTC	Alfatradiol	2002017	25118SI	40
Euro OTC	Alfatradiol	2006005	25473SI	40
Euro OTC	Alfatradiol	2103003	25689SI	50
Euro OTC	Alfatradiol	2201003	25948SI	40
Euro OTC	Alfatradiol	2301040	26601SI	40
Euro OTC	Alfatradiol	2305010	26755SI	40
Euro OTC	Alfatradiol	2305011	26756SI	40
Euro OTC	Alfatradiol	2305012	26757SI	40
Euro OTC	Alfatradiol	2305013	26758SI	34
Euro OTC	Alfatradiol	2305014	26759SI	40
Euro OTC	Alfatradiol	2310012	26998SI	40
Euro OTC	Alfatradiol	2409001	27388SI	40
Euro OTC	Alfatradiol	2409008	27389SI	40
Fagron	Alfatradiol	15J27-B08-323877	22933SI[†]	40
Fagron	Alfatradiol	22I06-B02-222372	26390SI	40

- 200 430 spectra from a total of 4022 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 955 spectra from 446 *Apo-Ident* customers from 271 batches from the substance/substance group *Alfatradiol*.

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- Among them are spectra of independent samples from 262 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Alfatradiol	2103003-01	1
	Alfatradiol	21D20-F06-379262	1
	Alfatradiol	21D20-F06-379263	1
	Alfatradiol	22000052001	2
	Alfatradiol	22000052002	1
	Alfatradiol	2200052001	1
	Alfatradiol	22A10-F02-381369	2
	Alfatradiol	22I06-B02-222371	1
	Alfatradiol	23000344003	1
	Alfatradiol	23000344004	2
	Alfatradiol	23000346002	4
	Alfatradiol	2301040-01	1
	Alfatradiol	24J10-B13-003480	1
	Alfatradiol	f02-3813609	1
Alliance	Alfatradiol	19159803	1
Anzag / Gehe	Alfatradiol	14C20-B02-294943	1
Audor Pharma	Alfatradiol	1617M-03305	1
Audor Pharma	Alfatradiol	18C23-B05-352725	1
Audor Pharma	Alfatradiol	2019Q-03305	1
Audor Pharma	Alfatradiol	2818A-03305	1
Audor Pharma	Alfatradiol	33-16-I-62P2985A	1
Audor Pharma	Alfatradiol	33-18-I-68P3620A	1
Audor Pharma	Alfatradiol	AP1404001-01A	1
Audor Pharma	Alfatradiol	AP1404001-01-A	1
Audor Pharma	Alfatradiol	AP1504015-01A	6
Audor Pharma	Alfatradiol	AP21-16-II-14P4511	2
Audor Pharma	Alfatradiol	AP21-16II-14P4511A	1
Audor Pharma	Alfatradiol	AP21-16-II-14P4511A	9
Audor Pharma	Alfatradiol	ap2116ll14p4511a	1
Audor Pharma	Alfatradiol	AP33_16_I_62P2985A	1
Audor Pharma	Alfatradiol	AP3316I42P2945A	1
Audor Pharma	Alfatradiol	AP33-16-I-42P2945A	4
Audor Pharma	Alfatradiol	AP3316I62P2985A	1
Audor Pharma	Alfatradiol	AP33-16-I-62P2985A	4
Audor Pharma	Alfatradiol	AP33-18-I68P3620A	1
Audor Pharma	Alfatradiol	AP33-18-I-68P3620A	6
Audor Pharma	Alfatradiol	AP35_17_II_85P3624A	1
Audor Pharma	Alfatradiol	AP35-17-II-85P3524A	1
Audor Pharma	Alfatradiol	AP35-17-II-85P3624	2
Audor Pharma	Alfatradiol	AP35-17-II-85P3624-1A	2
Audor Pharma	Alfatradiol	ap35-17-II-85P3624A	1
Audor Pharma	Alfatradiol	AP35-17-II-85P3624A	4
Audor Pharma	Alfatradiol	AP5100461A	2
Audor Pharma	Alfatradiol	AP5104925A	6
Audor Pharma	Alfatradiol	AP514925A	1
Audor Pharma	Alfatradiol	APXP103DAA	2
Audor Pharma	Alfatradiol	APXPC0071A	2
Bombastus	Alfatradiol	16G05-B01-335789	1
cae	Alfatradiol	20002390006	1
Caelo	Alfatradiol	10319904	1
Caelo	Alfatradiol	10319909	1
Caelo	Alfatradiol	11061001	2
Caelo	Alfatradiol	11061004	1
Caelo	Alfatradiol	11061005	1
Caelo	Alfatradiol	111161607	1
Caelo	Alfatradiol	11161805	4
Caelo	Alfatradiol	11161807	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Alfatradiol	12164201	4
Caelo	Alfatradiol	12164207	7
Caelo	Alfatradiol	12H29-N05	2
Caelo	Alfatradiol	13130805	5
Caelo	Alfatradiol	13130806	2
Caelo	Alfatradiol	13130808	1
Caelo	Alfatradiol	13201605	2
Caelo	Alfatradiol	14037904	3
Caelo	Alfatradiol	14130104	1
Caelo	Alfatradiol	14139102	3
Caelo	Alfatradiol	14139103	6
Caelo	Alfatradiol	14139104	14
Caelo	Alfatradiol	14139105	2
Caelo	Alfatradiol	14318502	2
Caelo	Alfatradiol	14318509	1
Caelo	Alfatradiol	14318511	3
Caelo	Alfatradiol	14318512	3
Caelo	Alfatradiol	14318514	2
Caelo	Alfatradiol	14C20-B02-294943	2
Caelo	Alfatradiol	14C20-B02-294944	1
Caelo	Alfatradiol	14I22-B30-302019	1
Caelo	Alfatradiol	15356801	16
Caelo	Alfatradiol	15356804	8
Caelo	Alfatradiol	1536801	1
Caelo	Alfatradiol	15380001	9
Caelo	Alfatradiol	15G07-B01-310227	1
Caelo	Alfatradiol	15G07-B01-311881	1
Caelo	Alfatradiol	16087501	12
Caelo	Alfatradiol	16087502	7
Caelo	Alfatradiol	16087504	22
Caelo	Alfatradiol	16087507	1
Caelo	Alfatradiol	16087510	3
Caelo	Alfatradiol	160875105728	1
Caelo	Alfatradiol	16087511	2
Caelo	Alfatradiol	16087512	9
Caelo	Alfatradiol	16180406	4
Caelo	Alfatradiol	16180408	7
Caelo	Alfatradiol	16180409	19
Caelo	Alfatradiol	16180412	1
Caelo	Alfatradiol	16180413	2
Caelo	Alfatradiol	16180415	2
Caelo	Alfatradiol	16G05-B01-335789	1
Caelo	Alfatradiol	16G05-B01-337353	1
Caelo	Alfatradiol	16G-B01-328254	1
Caelo	Alfatradiol	17G03-B11-341398	1
Caelo	Alfatradiol	18180409	1
Caelo	Alfatradiol	18C23-B05-354802	1
Caelo	Alfatradiol	19159801	4
Caelo	Alfatradiol	19159802	5
Caelo	Alfatradiol	19159803	10
Caelo	Alfatradiol	19159804	20
Caelo	Alfatradiol	19159805	6
Caelo	Alfatradiol	191599002	1
Caelo	Alfatradiol	191599003	10
Caelo	Alfatradiol	191599005	7
Caelo	Alfatradiol	19A24-B03-360709	1
Caelo	Alfatradiol	19K06-F04	1
Caelo	Alfatradiol	20002390001	1
Caelo	Alfatradiol	20002390003	11
Caelo	Alfatradiol	20002390006	14

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Alfatradiol	20004170001	1
Caelo	Alfatradiol	20004170003	2
Caelo	Alfatradiol	20004170004	9
Caelo	Alfatradiol	20004170006	6
Caelo	Alfatradiol	20004170009	5
Caelo	Alfatradiol	2000417001	1
Caelo	Alfatradiol	2000417004	2
Caelo	Alfatradiol	2061504	1
Caelo	Alfatradiol	21D20-F06-378303	1
Caelo	Alfatradiol	220000053005	2
Caelo	Alfatradiol	22000052001	6
Caelo	Alfatradiol	22000052002	8
Caelo	Alfatradiol	22000053003	2
Caelo	Alfatradiol	22000053004	4
Caelo	Alfatradiol	22000053005	14
Caelo	Alfatradiol	23000346006	1
Caelo	Alfatradiol	2830	1
Caelo	Alfatradiol	4318512	1
Caelo	Alfatradiol	5051406	1
Caelo	Alfatradiol	5107516	1
Caelo	Alfatradiol	511211	1
Caeol/Noweda	Alfatradiol	16180410	1
Caesar & Loretz GmbH...	Alfatradiol	19159803	1
Caesar & Loretz GmbH...	Alfatradiol	20002390004	1
Caesar & Loretz GmbH...	Alfatradiol	20002390003	1
Caesar & Loretz GmbH/AEP	Alfatradiol	20002390004	1
Caesar & Loretz GmbH/all	Alfatradiol	191599003	1
Caesar & Loretz GmbH/GEHE	Alfatradiol	20002390006	1
Caesar & Loretz GmbH/Gehe	Alfatradiol	22000052002	1
Caesar & Loretz GmbH...	Alfatradiol	20004170006	1
Caesar & Loretz GmbH/Kehr	Alfatradiol	22000052002	1
Caesar & Loretz GmbH...	Alfatradiol	19159804	1
Caesar & Loretz GmbH...	Alfatradiol	20F18-F01-372920	2
Caesar & Loretz GmbH/P	Alfatradiol	19159801	1
Caesar & Loretz GmbH/Sa	Alfatradiol	19159803	1
Caesar & Loretz GmbH...	Alfatradiol	19159805	1
Caesar & Loretz GmbH...	Alfatradiol	20004170004	1
Caesar & Loretz GmbH...	Alfatradiol	22000053005	1
Caesar & Loretz GmbH	Alfatradiol	16087512	1
Caesar & Loretz GmbH	Alfatradiol	16180407	1
Caesar & Loretz GmbH	Alfatradiol	16180408	1
Caesar & Loretz GmbH	Alfatradiol	16180409	1
Caesar & Loretz GmbH	Alfatradiol	16180413	1
Caesar & Loretz GmbH	Alfatradiol	19159801	2
Caesar & Loretz GmbH	Alfatradiol	19159803	4
Caesar & Loretz GmbH	Alfatradiol	19159804	2
Caesar & Loretz GmbH	Alfatradiol	19159805	2
Caesar & Loretz GmbH	Alfatradiol	191599002	1
Caesar & Loretz GmbH	Alfatradiol	191599003	5
Caesar & Loretz GmbH	Alfatradiol	191599005	7
Caesar & Loretz GmbH	Alfatradiol	20002390003	3
Caesar & Loretz GmbH	Alfatradiol	20002390004	1
Caesar & Loretz GmbH	Alfatradiol	20002390006	3
Caesar & Loretz GmbH	Alfatradiol	20004170001	2
Caesar & Loretz GmbH	Alfatradiol	20004170004	5
Caesar & Loretz GmbH	Alfatradiol	20004170006	5
Caesar & Loretz GmbH	Alfatradiol	20004170009	3
Caesar & Loretz GmbH	Alfatradiol	22000052002	4
Caesar & Loretz GmbH	Alfatradiol	22000052003	2
Caesar & Loretz GmbH	Alfatradiol	22000053003	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Alfatradiol	22000053004	1
Caesar & Loretz GmbH	Alfatradiol	22000053005	4
Caesar & Loretz GmbH	Alfatradiol	AP33-18-I-68P3620A	1
Caesar & Loretz/Sanacorp	Alfatradiol	16180409	1
Caesar und Loretz GmbH	Alfatradiol	16087502	1
Caesar&Lorenz/Phoenix	Alfatradiol	16087502	1
Caesar&Loretz GmbH/Anzag	Alfatradiol	12164207	1
Caesar/Lorenz	Alfatradiol	11061001	1
carlo	Alfatradiol	10319903	1
Chiracon GmbH	Alfatradiol	AP35-17-II-85P3624	1
Chiracon/Phoenix	Alfatradiol	35-19-I-14P3693	1
Euro OTC	Alfatradiol	121696	1
Euro OTC	Alfatradiol	1404001-01	2
Euro OTC	Alfatradiol	1404001-02	1
Euro OTC	Alfatradiol	15356804	1
Euro OTC	Alfatradiol	160301901	1
Euro OTC	Alfatradiol	1603019-03	3
Euro OTC	Alfatradiol	16087510	2
Euro OTC	Alfatradiol	16180410	1
Euro OTC	Alfatradiol	2002017-01	1
Euro OTC	Alfatradiol	200201702	1
Euro OTC	Alfatradiol	2002017-02	2
Euro OTC	Alfatradiol	20060005-01	1
Euro OTC	Alfatradiol	2006005-01	3
Euro OTC	Alfatradiol	2103003-01	7
Euro OTC	Alfatradiol	2201003-01	9
Euro OTC	Alfatradiol	2201830-01	1
Euro OTC	Alfatradiol	2209016-01	1
Euro OTC	Alfatradiol	2301040-01	1
Euro OTC	Alfatradiol	AP21-16-II-14P4511A	1
Euro OTC	Alfatradiol	AP33-16-I-62P2985A	1
Euro OTC	Alfatradiol	AP33-16-l-62P2985A	1
Fagron	Alfatradiol		2
Fagron	Alfatradiol	11B07-N05	1
Fagron	Alfatradiol	11D07-N19	1
Fagron	Alfatradiol	11G22-N11	2
Fagron	Alfatradiol	11k25-N01	1
Fagron	Alfatradiol	11K25-N01	3
Fagron	Alfatradiol	12D19-N03	6
Fagron	Alfatradiol	12H29-N05	4
Fagron	Alfatradiol	12J27-B08-314546	1
Fagron	Alfatradiol	12L19-N08	9
Fagron	Alfatradiol	12L19-No8	1
Fagron	Alfatradiol	13201605	1
Fagron	Alfatradiol	1372918	1
Fagron	Alfatradiol	13G19-N06	19
Fagron	Alfatradiol	13G19-N06	1
Fagron	Alfatradiol	13G19-N09	1
Fagron	Alfatradiol	13G19-No6	2
Fagron	Alfatradiol	13L30B32	1
Fagron	Alfatradiol	13L30-B32	2
Fagron	Alfatradiol	13L30-B32-290739	1
Fagron	Alfatradiol	13L30B32-290741	1
Fagron	Alfatradiol	13l30b32290742	1
Fagron	Alfatradiol	13L30-B32-290742	1
Fagron	Alfatradiol	14/22-B30-302017	3
Fagron	Alfatradiol	14722-B30-302018	1
Fagron	Alfatradiol	14C20-B02-294943	4
Fagron	Alfatradiol	14C20-B02-294944	1
Fagron	Alfatradiol	14G07-B99	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Alfatradiol	14G07-B99-294942	1
Fagron	Alfatradiol	14G07-B99-294945	4
Fagron	Alfatradiol	14I22-B30	1
Fagron	Alfatradiol	15G07-B01	1
Fagron	Alfatradiol	15G07-B01-310227	5
Fagron	Alfatradiol	15G07-B01-310228	3
Fagron	Alfatradiol	15G07-B01-310229	3
Fagron	Alfatradiol	15G07-B01-311881	2
Fagron	Alfatradiol	15J27-B08	1
Fagron	Alfatradiol	15J27-B08-314546	1
Fagron	Alfatradiol	15J27B08318164	1
Fagron	Alfatradiol	15J27-B08-318164	3
Fagron	Alfatradiol	15J27-B08-318783	1
Fagron	Alfatradiol	15J27-B08-321786	2
Fagron	Alfatradiol	16G05-801	1
Fagron	Alfatradiol	16g05-b01-324614	1
Fagron	Alfatradiol	16G05-B01-324614	1
Fagron	Alfatradiol	16G05-B01-325108	1
Fagron	Alfatradiol	16G05-B01-326866	1
Fagron	Alfatradiol	16G05-B01-328254	1
Fagron	Alfatradiol	16G05-B01-332379	4
Fagron	Alfatradiol	16G05-B01-334055	3
Fagron	Alfatradiol	16G05-B01-335789	7
Fagron	Alfatradiol	16G05-B01-337352	3
Fagron	Alfatradiol	16G05-B01-337353	1
Fagron	Alfatradiol	16G05-Bo1-332379	1
Fagron	Alfatradiol	16G05-N01-335789	1
Fagron	Alfatradiol	17G03-B11	4
Fagron	Alfatradiol	17G03-B11_348862	1
Fagron	Alfatradiol	17G03-B11-341398	2
Fagron	Alfatradiol	17G03-B11-341399	2
Fagron	Alfatradiol	17G03-B11-345093	5
Fagron	Alfatradiol	17G03-B11-346962	1
Fagron	Alfatradiol	17G03-B11-348862	2
Fagron	Alfatradiol	17G03-B11-348863	1
Fagron	Alfatradiol	18C23-B05	2
Fagron	Alfatradiol	18C23-B05_350996	1
Fagron	Alfatradiol	18C23-B05_354802	1
Fagron	Alfatradiol	18C23-B05-350996	4
Fagron	Alfatradiol	18C23-B05-352724	2
Fagron	Alfatradiol	18C23-B05-352725	1
Fagron	Alfatradiol	18C23-B05-354802	9
Fagron	Alfatradiol	18C23-B05-356316	2
Fagron	Alfatradiol	18C23-B05-4802	1
Fagron	Alfatradiol	19A24-B003360712	1
Fagron	Alfatradiol	19A24-B03	3
Fagron	Alfatradiol	19A24-B03_360710	1
Fagron	Alfatradiol	19A24-B03-360709	3
Fagron	Alfatradiol	19A24-B03-360710	13
Fagron	Alfatradiol	19AB03360709	1
Fagron	Alfatradiol	19K06-F04	1
Fagron	Alfatradiol	19K06F04366005	1
Fagron	Alfatradiol	19K06-F04-366005	10
Fagron	Alfatradiol	19K06-F04-366006	2
Fagron	Alfatradiol	19K06-F04-366007	2
Fagron	Alfatradiol	20122-F02-374255	2
Fagron	Alfatradiol	20122-F02-374256	1
Fagron	Alfatradiol	20F18-F01	1
Fagron	Alfatradiol	20F18F01372918	2
Fagron	Alfatradiol	20F18-F01-372918	15

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Alfatradiol	20F18-F01372920	1
Fagron	Alfatradiol	20F18-F01-372920	2
Fagron	Alfatradiol	20F8-FD1	1
Fagron	Alfatradiol	20I22-F02-374255	3
Fagron	Alfatradiol	20I22-F02-374256	2
Fagron	Alfatradiol	21D20_F06_379262	1
Fagron	Alfatradiol	21D20-F036-379262	1
Fagron	Alfatradiol	21D20-F06	2
Fagron	Alfatradiol	21D20F06378303	2
Fagron	Alfatradiol	21D20-F06-378303	6
Fagron	Alfatradiol	21D20-F06-378305	2
Fagron	Alfatradiol	21D20-F06-378306	2
Fagron	Alfatradiol	21D20-F06-378476	3
Fagron	Alfatradiol	21d20f06379262	1
Fagron	Alfatradiol	21D20-F06-379262	10
Fagron	Alfatradiol	21D20-F06-379263	2
Fagron	Alfatradiol	22A10-F02-381369	7
Fagron	Alfatradiol	22A10-F02-381421	1
Fagron	Alfatradiol	23E15-B08-224470	1
Fagron	Alfatradiol	2735	1
Fagron	Alfatradiol	324614	1
Fagron	Alfatradiol	5102432	1
Fagron	Alfatradiol	5111184	2
Fagron	Alfatradiol	5115018	1
Fagron	Alfatradiol	5119507	4
Fagron	Alfatradiol	5122243	6
Fagron	Alfatradiol	5122244	1
Fagron	Alfatradiol	6882484	1
Fagron	Alfatradiol	9011904	1
Fagron	Alfatradiol	F01-3729103	1
Fagron	Alfatradiol	F04-3660005	1
Fagron	Alfatradiol	F04-3660006	1
Fagron	Alfatradiol	F0637926002	1
Fagron	Alfatradiol	XP101UT	1
Fargon/AHD	Alfatradiol	17G03-B11	1
Fargon/Kehr	Alfatradiol	16G05-B01-332379	1
Fargon	Alfatradiol	21D20-F06-379262	1
Fgron / Alliance Healthc.	Alfatradiol	16G05-B01-328254	1
Fiebig/Farago	Alfatradiol	19A24-B03-360709	1
fragon/phonix	Alfatradiol	17G03-B11-341399	1
Gatt-Koller	Alfatradiol	180077661	1
Gatt-Koller	Alfatradiol	1803210	2
Gehe/Fragron	Alfatradiol	5111184	2
Gehe	Alfatradiol	16087501	1
GEHE	Alfatradiol	16087512	1
Gehe	Alfatradiol	19159801	1
Gehe	Alfatradiol	22000053007	1
gepepharm/Phoenix	Alfatradiol	19054203	2
Kehr	Alfatradiol	18C23-B05-350996	1
Kehr	Alfatradiol	19KO6-FO4-3660055	1
Kwizda	Alfatradiol	529068	1
Noweda am 10.08.2018	Alfatradiol	16087510	1
Noweda/Fragron	Alfatradiol	16G05-B01-332379	1
Noweda	Alfatradiol	16G05-B01-324614	2
Noweda	Alfatradiol	19159803	1
Noweda	Alfatradiol	21D20-F06-378303	1
Noweda	Alfatradiol	22000053007	1
Noweda	Alfatradiol	22A10-F02-381369	1
Noweda	Alfatradiol	2301040-01	1
Phönix	Alfatradiol	15356801	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Alfatradiol	21D20-F06-378305	1
Phönix	Alfatradiol	33-18-1-68P3620A	1
Phönix	Alfatradiol	APXPC0071A	1
Phönix	Alfatradiol	B05-3509906	1
Proquina / Gehe	Alfatradiol	15356801	1
Proquina / Gehe	Alfatradiol	19A24-B03-360711	1
Proquina / Gehe	Alfatradiol	5122243	1
Proquina / Gehe	Alfatradiol	6882478	1
Proquina / Gehe	Alfatradiol	F04-3660006	1
Proquina / Sanacorp	Alfatradiol	F04-3660005	1
Sanacorp, 39,57EUR, 27.1.17	Alfatradiol	700670-0011	1
Sanacorp	Alfatradiol	13201605	1
Sanacorp	Alfatradiol	15356804	1
Sanacorp	Alfatradiol	19159802	2
Sanacorp	Alfatradiol	2103003-01	1
Sanacorp	Alfatradiol	21D20-F06-379262	1
Sanacorp	Alfatradiol	22A10-F02-381369	1
Shandong Northwest M...	Alfatradiol	AEC160522	1
Shandong northwest m...	Alfatradiol	AEC151211	1
VDL 1.7.14;40.30 euro	Alfatradiol	13G19-N06	1

- 235 112 spectra from 1515 *Apo-Ident* customers from a total of 48 991 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	810	0	152 152
Type B	0	1654	0	200 430
Type C	0	941	14	235 112

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.2593 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.6372 %)
Type C	100.0000 % (> 99.9007 %)	98.5340 % (> 98.2199 %)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20940	20940	0.00	115.46
21476	22511	22.09	125.52
21477	22511	24.74	124.97
21714	21714	0.00	122.09
22511	22511	0.00	119.66
22933	22511	9.60	120.08
22934	22511	5.03	119.49
22935	25553	9.42	131.49
24662	24747	40.23	128.00
24747	24747	0.00	128.70
25553	25553	0.00	130.55
25561	25561	0.00	129.02

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Allantoin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20079-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Allantoin; Allantoinum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Allantoin	7	7	123

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	110.92	–

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Allantoin	162289	22756	40	20160815*
Caelo	Allantoin	172346	23629	40	20171019*
Caelo	Allantoin	172346	23635	40	20171019*
Euro OTC	Allantoin	1406011-01	21625	60	20140718
Euro OTC	Allantoin	1609012	22750	40	20161006*
Euro OTC	Allantoin	1609012-01	22810	40	20161006
Euro OTC	Allantoin	1406011-04	24095	40	20170213
Fagron	Allantoin	13I03-B05	21216	40	20130927

Validation samples

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

Type A All calibration spectra.

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 340 spectra of 8 reference samples from the substance/substance group *Allantoin*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 622 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 330 spectra of 9 reference samples from the substance/substance group *Allantoin*.

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

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Allantoin	181586	24235	40
Caelo	Allantoin	191828	24894	40
Caelo	Allantoin	21003135	25848	50
Caelo	Allantoin	23000841	27337	40
Euro OTC	Allantoin	1811006	24344	40
Euro OTC	Allantoin	2101022	25593	40
Euro OTC	Allantoin	2212010	26511	40
Caelo	Allantoin	23000841	27337SI	20
Euro OTC	Allantoin	2212010	26511SI	20

- 201 754 spectra from a total of 4038 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 564 spectra from 256 *Apo-Ident* customers from 126 batches from the substance/substance group *Allantoin*.

- Among them are spectra of independent samples from 123 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Allantoin	20004526005	1
	Allantoin	21003135003	1
	Allantoin	21003135007	1
	Allantoin	21003135015	1
ACM Herba	Allantoin	22J00443	1
AHD	Allantoin	1609012-01	1
Anzag;18.03.15;2,76EUR	Allantoin	14247602	1
Caelo	Allantoin	10064008	4
Caelo	Allantoin	10064012	1
Caelo	Allantoin	10064015	1
Caelo	Allantoin	10318305	1
Caelo	Allantoin	10318312	1
Caelo	Allantoin	10318313	2
Caelo	Allantoin	1113E-01087	1
Caelo	Allantoin	11247504	5
Caelo	Allantoin	11247510	2
Caelo	Allantoin	11247511	2
Caelo	Allantoin	121127	1
Caelo	Allantoin	1225101	1
Caelo	Allantoin	12251501	4
Caelo	Allantoin	12251502	2
Caelo	Allantoin	12251505	7
Caelo	Allantoin	12251510	9
Caelo	Allantoin	12251511	1
Caelo	Allantoin	12374401	1
Caelo	Allantoin	12374403	8
Caelo	Allantoin	12374404	2
Caelo	Allantoin	12374407	4
Caelo	Allantoin	12374408	1
Caelo	Allantoin	12374409	15
Caelo	Allantoin	12374414	8
Caelo	Allantoin	12374415	10
Caelo	Allantoin	12374417	1
Caelo	Allantoin	12374418	2
Caelo	Allantoin	12374422	9
Caelo	Allantoin	12374423	2
Caelo	Allantoin	1251505	1
Caelo	Allantoin	140512	1
Caelo	Allantoin	1406011-05	1
Caelo	Allantoin	14247602	6
Caelo	Allantoin	14247609	10
Caelo	Allantoin	14247610	1
Caelo	Allantoin	1522000	1
Caelo	Allantoin	152200012	1
Caelo	Allantoin	15220004	1
Caelo	Allantoin	15220005	2
Caelo	Allantoin	15220006	17
Caelo	Allantoin	15220007	4
Caelo	Allantoin	15220008	11
Caelo	Allantoin	15220010	3
Caelo	Allantoin	15220011	2
Caelo	Allantoin	15220012	11
Caelo	Allantoin	1522008	1
Caelo	Allantoin	15275302	1
Caelo	Allantoin	15275304	3
Caelo	Allantoin	15275305	3
Caelo	Allantoin	15275312	8
Caelo	Allantoin	16228903	13
Caelo	Allantoin	16228904	1
Caelo	Allantoin	16228906	17

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Allantoin	16228913	2
Caelo	Allantoin	16228914	3
Caelo	Allantoin	16228915	28
Caelo	Allantoin	17355901	2
Caelo	Allantoin	17355903	20
Caelo	Allantoin	17355904	1
Caelo	Allantoin	17355905	1
Caelo	Allantoin	1811006-01	1
Caelo	Allantoin	18158602	12
Caelo	Allantoin	18158604	12
Caelo	Allantoin	18158605	4
Caelo	Allantoin	18158606	1
Caelo	Allantoin	18158613	3
Caelo	Allantoin	1918202	1
Caelo	Allantoin	191828002	2
Caelo	Allantoin	19182802	1
Caelo	Allantoin	19182803	7
Caelo	Allantoin	20002009004	7
Caelo	Allantoin	20004518002	3
Caelo	Allantoin	20004518003	8
Caelo	Allantoin	20004526003	7
Caelo	Allantoin	20004526005	5
Caelo	Allantoin	20004526006	1
Caelo	Allantoin	2004526005	1
Caelo	Allantoin	20071202	1
Caelo	Allantoin	20140612-15	1
Caelo	Allantoin	21003135003	1
Caelo	Allantoin	21003135007	5
Caelo	Allantoin	2100315007	1
Caelo	Allantoin	2264594	1
Caelo	Allantoin	2713431	1
Caelo	Allantoin	2713448	1
Caelo	Allantoin	28101702	1
Caelo	Allantoin	4247602	1
Caelo	Allantoin	5051402	1
Caelo	Allantoin	81542099	1
Caelo	Allantoin	81542358	2
Caesar & Loretz GmbH...	Allantoin	17355905	2
Caesar & Loretz GmbH...	Allantoin	191828002	1
Caesar & Loretz GmbH...	Allantoin	18158605	1
Caesar & Loretz GmbH...	Allantoin	191828002	1
Caesar & Loretz GmbH...	Allantoin	20002009004	1
Caesar & Loretz GmbH...	Allantoin	18158604	2
Caesar & Loretz GmbH...	Allantoin	20002009004	1
Caesar & Loretz GmbH...	Allantoin	18158604	1
Caesar & Loretz GmbH	Allantoin	12251505	1
Caesar & Loretz GmbH	Allantoin	12251510	1
Caesar & Loretz GmbH	Allantoin	12374403	1
Caesar & Loretz GmbH	Allantoin	12374409	1
Caesar & Loretz GmbH	Allantoin	12374415	1
Caesar & Loretz GmbH	Allantoin	12374416	1
Caesar & Loretz GmbH	Allantoin	14247602	1
Caesar & Loretz GmbH	Allantoin	18158602	2
Caesar & Loretz GmbH	Allantoin	18158604	3
Caesar & Loretz GmbH	Allantoin	18158605	1
Caesar & Loretz GmbH	Allantoin	18158613	2
Caesar & Loretz GmbH	Allantoin	191828002	4
Caesar & Loretz GmbH	Allantoin	19182803	4
Caesar & Loretz GmbH	Allantoin	20004518002	1
Caesar & Loretz GmbH	Allantoin	20004518003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
CAESAR & LORETZ GMBH	Allantoin	20004526005	1
Caesar & Loretz GmbH	Allantoin	21003135007	1
Caesar & Loretz Hilden	Allantoin	17355903	1
Caesar & Loretz	Allantoin	16228906	1
Caesar&Loretz GmbH	Allantoin	12374409	1
Caeser / Gehe	Allantoin	15220007	1
Cealo/Phönix	Allantoin	18158602	1
celo/Jenne	Allantoin	12374403	1
Deretil SA / Allianc...	Allantoin	2101022-01	1
DSM Nutritional Prod...	Allantoin	12251505	1
EuRho / Phoenix	Allantoin	1406011-03	1
EuRho	Allantoin	1406011-04	1
Euro OTC	Allantoin	140104601	1
Euro OTC	Allantoin	1401046-01	3
Euro OTC	Allantoin	1406011	2
Euro OTC	Allantoin	1406011-01	7
Euro OTC	Allantoin	1406011-02	3
Euro OTC	Allantoin	140601103	1
Euro OTC	Allantoin	1406011-04	1
Euro OTC	Allantoin	1406011-05	3
Euro OTC	Allantoin	15220008	2
Euro OTC	Allantoin	1609012-01	10
Euro OTC	Allantoin	160901202	1
Euro OTC	Allantoin	1609012-02	3
Euro OTC	Allantoin	1609012-03	2
Euro OTC	Allantoin	16228915	1
Euro OTC	Allantoin	18110006-01	1
Euro OTC	Allantoin	1811006	1
Euro OTC	Allantoin	1811006-01	11
Euro OTC	Allantoin	181100602	1
Euro OTC	Allantoin	1811006-02	11
Euro OTC	Allantoin	1811006-03	8
Euro OTC	Allantoin	2101022-01	8
Euro OTC	Allantoin	5024-000077	1
Euro OTC	Allantoin	K93504015	1
Fagron	Allantoin	11J11-N11	3
Fagron	Allantoin	12B09-N09	1
Fagron	Allantoin	12C30-N04	1
Fagron	Allantoin	13A21-N07	3
Fagron	Allantoin	13G16-N07	6
Fagron	Allantoin	13I03-B05-289430	1
Fagron	Allantoin	16228905	2
Fagron	Allantoin	5011E-01087	1
Fargron/AHD	Allantoin	13G16-N07	1
Gehe	Allantoin	12251510	1
Gehe	Allantoin	14247603	1
Gehe	Allantoin	15220008	1
Gehe	Allantoin	15220012	1
Gehe	Allantoin	1609012-02	1
Gehe	Allantoin	17355903	1
Gehe	Allantoin	1811006-02	1
Herba Chemosan	Allantoin	22JOD443	1
Ichthyol-Gesellschaft	Allantoin	16228915	1
Kehr	Allantoin	15220008	1
Krieger/Hedinger	Allantoin	15220006	1
Merck	Allantoin	1406011-05	1
Merck	Allantoin	160901201	1
Merck	Allantoin	1609012-01	1
Noweda	Allantoin	1609012-01	1
Noweda	Allantoin	16228915	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Allantoin	21003135015	1
Noweda	Allantoin	2101022-02	1
Phoenix 08.10.14	Allantoin	1401046-01	1
Sanacorp	Allantoin	12251501	1
Sanacorp	Allantoin	12251510	1
Sanacorp	Allantoin	12374409	2
Sanacorp	Allantoin	12374422	1
Sanacorp	Allantoin	15275312	1
Sanacorp	Allantoin	1811006-02	1
Sanacorp	Allantoin	K93504015	1
Spinnrad	Allantoin	1217503012	1
VDL 17.10.14	Allantoin	12374415	1

- 235 503 spectra from 1515 *Apo-Ident* customers from a total of 49 132 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	340	0	152 622
Type B	0	330	0	201 754
Type C	0	562	2	235 503

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2353 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.1818 %)
Type C	100.0000 % (> 99.9007 %)	99.6454 % (> 99.1135 %)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21216	22756	10.19	288.39
21625	22750	9.93	288.78
22750	22750	0.00	283.25
22756	22756	0.00	276.82
22810	22750	6.04	278.41
23629	23629	0.00	274.08
23635	23635	0.00	275.83
24095	22750	6.28	281.58

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Allopurinol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	22243-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Allopurinol; Allopurinolum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Allopurinol	4	2	17

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Glycine	112.68	–

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Allopurinol	14E15-B05-307746	22243	60	AR-16-FG-004367-01
Fagron	Allopurinol	14E15-B05-315557	22345	60	20140611
Fagron	Allopurinol	14E15-B05-307746	22836	40	20140611
Fagron	Allopurinol	22H29-B06-223774	26450	40	20220930
Fagron	Allopurinol	23D12-B06-228657	26818	40	20230510

Validation samples

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

Type A All calibration spectra.

- 240 spectra of 5 reference samples from the substance/substance group *Allopurinol*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 722 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

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

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

- 160 spectra of 5 reference samples from the substance/substance group *Allopurinol*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Allopurinol	14E15-B05-330859	23523	40
Fagron	Allopurinol	18E23-B02-357777	24577	40
Fagron	Allopurinol	14E15-B05-330859	23526	40
Fagron	Allopurinol	22H29-B06-223774	26450SI†	20
Fagron	Allopurinol	23D12-B06-228657	26818SI†	20

- 201 924 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 38 spectra from 19 *Apo-Ident* customers from 19 batches from the substance/substance group *Allopurinol*.
- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Allopurinol	18E23-B02-350905	1
Fagron	Allopurinol	14E15-B05_315557	1
Fagron	Allopurinol	14E15-B05-315557	14
Fagron	Allopurinol	14E15B05-320787	1
Fagron	Allopurinol	14E15-B05-320787	1
Fagron	Allopurinol	14E15-B05-337862	4
Fagron	Allopurinol	14E15-B08	1

continued on the next page

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

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Allopurinol	18E23-B02	1
Fagron	Allopurinol	18E23-B02-350905	1
Fagron	Allopurinol	18E23-B02-357777	3
Fagron	Allopurinol	18E23-B02-361600	1
Fagron	Allopurinol	190261502	1
Fagron	Allopurinol	19061206	1
Fagron	Allopurinol	200250306	1
Fagron	Allopurinol	200803107	1
Fagron	Allopurinol	22H29-B06-223774	1
Fagron	Allopurinol	B02-3509005	1
Fagron	Allopurinol	B02-3577707	1
Fagron	Allopurinol	B02-3616000	1
Phönix	Allopurinol	200612506	1

- 236 029 spectra from 1515 *Apo-Ident* customers from a total of 49 240 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	240	0	152 722
Type B	0	160	0	201 924
Type C	0	38	0	236 029

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 84.2105 %)

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

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

Identity according to identity test using NIR spectroscopy

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22243	22243	0.00	190.96
22345	22243	3.54	193.07
22836	22243	4.08	194.26
26450	22243	8.29	194.35
26818	22243	15.00	194.55

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**alpha-tocopheryl acetate dry concentrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20433-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

alpha-tocopheryl acetate dry concentrate; alpha-Tocopherylis acetatis pulvis

Special notes

When selecting the *alpha-tocopheryl acetate dry concentrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
alpha-tocopheryl acetate dry concentrate	10	10	23

Second-stage model

For differentiation of the substance/substance group *alpha-tocopheryl acetate dry concentrate* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Nystatin	64.60	27.61
⋮	⋮	⋮
Bacitracin	>50	18.72
Amphotericin B	>50	35.80
Polymyxin B sulfate	76.78	41.80
Colistin sulfate	>50	46.14
Selenium yeast	>50	50.17
Cyanocobalamin	>50	53.39
Estriol	>50	62.11
Estradiol hemihydrate	>50	63.89
Riboflavin	>50	68.54
Calcium glycerophosphate	>50	77.14
Triamcinolone	>50	91.34
Carmellose sodium	>50	101.48
Calcium pantothenate	>50	122.62
Gelatine, white	>50	145.58
Methylcobalamin	>50	169.20
SyrSpend® SF Alka	>50	178.21
Hyoscine hydrobromide	>50	181.97
SyrSpend® SF pH4 neo (Maize starch)	>50	185.88
Tosylchloramide sodium	>50	187.50
Rice starch	>50	201.70
Corn starch	>50	263.04
Oxalic acid	>50	281.34
SyrSpend® SF pH4	>50	342.55
Acacia, dried dispersion	>50	370.10
Maltodextrin	>50	376.64
Wheat starch	>50	399.60
Potato starch	>50	417.15
Fructose	>50	631.69

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	alpha-tocopheryl acetate ...	1110021-02	20907	40	20120104
Euro OTC	alpha-tocopheryl acetate ...	1305032-01	21680	60	AR-15-FG-001194-01
Euro OTC	alpha-tocopheryl acetate ...	1507001	21842	60	20130708*
Euro OTC	alpha-tocopheryl acetate ...	1603046	22543	40	20160429*
Euro OTC	alpha-tocopheryl acetate ...	1907033	24841	40	20190820*
Euro OTC	alpha-tocopheryl acetate ...	2005022	25277	40	20200728*
Euro OTC	alpha-tocopheryl acetate ...	2101019	25599	40	20210323*
Fagron	alpha-tocopheryl acetate ...	13H30-B02-287169	21609	60	AR-15-FG-006388-01
Fagron	alpha-tocopheryl acetate ...	14B03-B04-295113	21959	60	20140224
Fagron	Vitamin E acetate powder 50%	022402A013	BR20042	40	20240919*
Fagron	Vitamin E acetate powder 50%	022402A013	BR20042SI	20	20240919*

Validation samples

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

Type A All calibration spectra.

- 500 spectra of 11 reference samples from the substance/substance group *alpha-tocopheryl - acetate dry concentrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.
- 152 462 spectra from a total of 2832 batches from further 482 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 510 spectra of 15 reference samples from the substance/substance group *alpha-tocopheryl - acetate dry concentrate*.
- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

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

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	alpha-tocopheryl acetate …	1705003	23424	40
Euro OTC	alpha-tocopheryl acetate …	1810024	24309	40
Euro OTC	alpha-tocopheryl acetate …	2106013	25780	50
Euro OTC	alpha-tocopheryl acetate …	2111015	25889	50
Euro OTC	alpha-tocopheryl acetate …	2207013	26279	40
Euro OTC	alpha-tocopheryl acetate …	2309007	26929	40
Euro OTC	alpha-tocopheryl acetate …	2408017	27395	40
Fagron	alpha-tocopheryl acetate …	16H30-B05-326792	22948	40
Fagron	Vitamin E acetate powder 50%	022403A011	BR20041	40
Fagron	Vitamin E acetate powder 50%	022402A012	BR20043	40
Euro OTC	alpha-tocopheryl acetate …	2111015	25889SI	10
Euro OTC	alpha-tocopheryl acetate …	2207013	26279SI	20
Euro OTC	alpha-tocopheryl acetate …	2309007	26929SI	20
Fagron	Vitamin E acetate powder 50%	022403A011	BR20041SI	20
Fagron	Vitamin E acetate powder 50%	022402A012	BR20043SI	20

- 201 574 spectra from a total of 4035 batches from further 837 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 44 spectra from 15 *Apo-Ident* customers from 25 batches from the substance/substance group *alpha-tocopheryl acetate dry concentrate*.

- Among them are spectra of independent samples from 23 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Bombastus	alpha-tocopheryl acetate …	1507001-02	1
Caelo	alpha-tocopheryl acetate …	1705003-01	1
EuRho	alpha-tocopheryl acetate …	1810024-01	1
Euro OTC	alpha-tocopheryl acetate …	1110021-02	2
Euro OTC	alpha-tocopheryl acetate …	1507001-01	2
Euro OTC	alpha-tocopheryl acetate …	160304602	1
Euro OTC	alpha-tocopheryl acetate …	1603046-02	3
Euro OTC	alpha-tocopheryl acetate …	170500301	1
Euro OTC	alpha-tocopheryl acetate …	1705003-01	1
Euro OTC	alpha-tocopheryl acetate …	1705003-02	1
Euro OTC	alpha-tocopheryl acetate …	1705003-04	2
Euro OTC	alpha-tocopheryl acetate …	1705003-05	1
Euro OTC	alpha-tocopheryl acetate …	181002401	1
Euro OTC	alpha-tocopheryl acetate …	1810024-01	4
Euro OTC	alpha-tocopheryl acetate …	190033-01	1
Euro OTC	alpha-tocopheryl acetate …	1907033-01	1
Euro OTC	alpha-tocopheryl acetate …	190703302	1
Euro OTC	alpha-tocopheryl acetate …	1907033-02	1
Euro OTC	alpha-tocopheryl acetate …	200502201	1
Euro OTC	alpha-tocopheryl acetate …	2005022-01	6
Euro OTC	alpha-tocopheryl acetate …	2106013-01	2
Euro OTC	alpha-tocopheryl acetate …	2111015-01	1
Euro OTC	alpha-tocopheryl acetate …	2207013-01	2
Euro/Sanacorp	alpha-tocopheryl acetate …	150700101	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	alpha-tocopheryl acetate …	13H30-B02-287169	1
Fagron	alpha-tocopheryl acetate …	16H30-B05-326792	1
Kehr	alpha-tocopheryl acetate …	1705003-03	2
Sanacorp	alpha-tocopheryl acetate …	1705003-03	1

- 236 023 spectra from 1515 *Apo-Ident* customers from a total of 49 234 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	500	0	152 462
Type B	0	468	42	201 574
Type C	0	44	0	236 023

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8000 %)
Type B	100.0000 % (> 99.9912 %)	91.7647 % (> 91.1765 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 86.3636 %)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20907	21680	7.03	116.28
21609	21609	0.00	116.63
21680	21680	0.00	119.79
21842	21842	0.00	118.52
21959	21680	11.27	131.82
22543	22543	0.00	123.37
24841	24841	0.00	144.83
25277	25277	0.00	126.67
25599	25599	0.00	136.21
BR20042	BR20042	0.00	83.15

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Aluminium chloride hexahydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20131-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Aluminium chloride hexahydrate; Aluminii chloridum hexahydricum

Special notes

When selecting the *Aluminium chloride hexahydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Aluminium chloride hexahydrate	6	3	130

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Menthol	102.91	–

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Aluminium chloride hexahydrate	22002438	26556	40	20221121*
Euro OTC	Aluminium chloride hexahydrate	1911008-03	26049	40	20210630
Euro OTC	Aluminium chloride hexahydrate	2207005	26203	40	20220726*
Euro OTC	Aluminium chloride hexahydrate	2207005	26203SI	20	20220726*
Fagron	Aluminium chloride hexahydrate	21F07-B18-213240	26059	40	20211105
Fagron	Aluminium chloride hexahydrate	23F22-B08-232244	27019	40	20230705
Fagron	Aluminium chloride hexahydrate	23K16-B03-234491	27059	40	20231130

Validation samples

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

Type A All calibration spectra.

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 260 spectra of 7 reference samples from the substance/substance group *Aluminium chloride hexahydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 150 spectra of 6 reference samples from the substance/substance group *Aluminium chloride hexahydrate*.

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

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Aluminium chloride hexahydrate	21002588	26053	40
Fagron	Aluminium chloride hexahydrate	12I27-N01	20903	40
Fagron	Aluminium chloride hexahydrate	23C23-B17-227778	26670	40
Caelo	Aluminium chloride hexahydrate	21002588	26053SI	10
Euro OTC	Aluminium chloride hexahydrate	1911008-03	26049SI†	10
Fagron	Aluminium chloride hexahydrate	21F07-B18-213240	26059SI†	10

- 201 934 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 534 spectra from 240 *Apo-Ident* customers from 138 batches from the substance/substance group *Aluminium chloride hexahydrate*.

- Among them are spectra of independent samples from 130 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

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

Supplier	Substance	Batch	Spectra
	Aluminium chloride hexahydrate	1911008-03	2
	Aluminium chloride hexahydrate	1911008-04	3
	Aluminium chloride hexahydrate	21002588002	1
	Aluminium chloride hexahydrate	21002588006	1
	Aluminium chloride hexahydrate	22002438001	11
	Aluminium chloride hexahydrate	22002438002	5
	Aluminium chloride hexahydrate	22002438003	1
	Aluminium chloride hexahydrate	22002438005	3
	Aluminium chloride hexahydrate	22002438006	6
	Aluminium chloride hexahydrate	22002438008	2
	Aluminium chloride hexahydrate	22002438010	7
	Aluminium chloride hexahydrate	22002438012	1
	Aluminium chloride hexahydrate	22002438013	1
	Aluminium chloride hexahydrate	220700501	1
	Aluminium chloride hexahydrate	2207005-01	18
	Aluminium chloride hexahydrate	2207005-02	4
	Aluminium chloride hexahydrate	22G29-B04	1
	Aluminium chloride hexahydrate	22K14-B01-225235	1
	Aluminium chloride hexahydrate	23c23-b17-227777	1
	Aluminium chloride hexahydrate	23C23-B17-227777	3
	Aluminium chloride hexahydrate	23k16-b03-234491	1
	Aluminium chloride hexahydrate	7784-13-6	1
	Aluminium chloride hexahydrate	K140A	1
5,56	Aluminium chloride hexahydrate	22002438010	1
AHD	Aluminium chloride hexahydrate	22002438001	1
AHD	Aluminium chloride hexahydrate	22002438002	1
AHD	Aluminium chloride hexahydrate	22002438012	1
AHD	Aluminium chloride hexahydrate	22K14-B01-225218	2
Alliance Healthcare	Aluminium chloride hexahydrate	13D22-N09	1
Alliance	Aluminium chloride hexahydrate	21F07-B18-213240	1
Anzag	Aluminium chloride hexahydrate	1204026-02	1
Caelo	Aluminium chloride hexahydrate		2
Caelo	Aluminium chloride hexahydrate	10251307	1
Caelo	Aluminium chloride hexahydrate	10251314	1
Caelo	Aluminium chloride hexahydrate	11229905	1
Caelo	Aluminium chloride hexahydrate	11229906	1
Caelo	Aluminium chloride hexahydrate	11229907	1
Caelo	Aluminium chloride hexahydrate	11229914	1
Caelo	Aluminium chloride hexahydrate	11229917	2
Caelo	Aluminium chloride hexahydrate	12021303	1
Caelo	Aluminium chloride hexahydrate	120402601	1
Caelo	Aluminium chloride hexahydrate	1204026-01	3
Caelo	Aluminium chloride hexahydrate	1204026-02	2
Caelo	Aluminium chloride hexahydrate	12047503	2
Caelo	Aluminium chloride hexahydrate	12047508	3
Caelo	Aluminium chloride hexahydrate	12047512	1
Caelo	Aluminium chloride hexahydrate	12047514	3
Caelo	Aluminium chloride hexahydrate	1210014-01	3
Caelo	Aluminium chloride hexahydrate	12114902	2
Caelo	Aluminium chloride hexahydrate	12114904	2
Caelo	Aluminium chloride hexahydrate	12114906	4
Caelo	Aluminium chloride hexahydrate	12114908	7
Caelo	Aluminium chloride hexahydrate	12114910	4
Caelo	Aluminium chloride hexahydrate	12114912	4
Caelo	Aluminium chloride hexahydrate	12114918	11
Caelo	Aluminium chloride hexahydrate	12114919	1
Caelo	Aluminium chloride hexahydrate	12114920	10
Caelo	Aluminium chloride hexahydrate	12114922	13
Caelo	Aluminium chloride hexahydrate	12323702	10
Caelo	Aluminium chloride hexahydrate	12323710	8

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Aluminium chloride hexahydrate	12323711	12
Caelo	Aluminium chloride hexahydrate	12323717	4
Caelo	Aluminium chloride hexahydrate	12C07-N01	2
Caelo	Aluminium chloride hexahydrate	12i27-N01	1
Caelo	Aluminium chloride hexahydrate	12I27-N01	1
Caelo	Aluminium chloride hexahydrate	12l27-N01	2
Caelo	Aluminium chloride hexahydrate	12l27-NO1	1
Caelo	Aluminium chloride hexahydrate	13/13-B03-287298	1
Caelo	Aluminium chloride hexahydrate	13D22-N09	3
Caelo	Aluminium chloride hexahydrate	13G03-N02	2
Caelo	Aluminium chloride hexahydrate	13L13-B03-287298	1
Caelo	Aluminium chloride hexahydrate	15051302	1
Caelo	Aluminium chloride hexahydrate	15080701	1
Caelo	Aluminium chloride hexahydrate	15080715	1
Caelo	Aluminium chloride hexahydrate	18061308	1
Caelo	Aluminium chloride hexahydrate	18261314	1
Caelo	Aluminium chloride hexahydrate	19041302	1
Caelo	Aluminium chloride hexahydrate	23111203	1
Caelo	Aluminium chloride hexahydrate	28121301	1
Caelo	Aluminium chloride hexahydrate	3091205	1
Caelo	Aluminium chloride hexahydrate	3113E-01095	1
Caelo	Aluminium chloride hexahydrate	5081301	1
Caelo	Aluminium chloride hexahydrate	51/AD1	1
Caelo	Aluminium chloride hexahydrate	8031301	1
Caelo	Aluminium chloride hexahydrate	9071303	1
Caelo	Aluminium chloride hexahydrate	C181A	1
Caesar & Loretz GmbH...	Aluminium chloride hexahydrate	12114918	4
Caesar & Loretz GmbH...	Aluminium chloride hexahydrate	12047508	1
Caesar & Loretz GmbH...	Aluminium chloride hexahydrate	12114906	1
Caesar & Loretz GmbH...	Aluminium chloride hexahydrate	12323702	1
Caesar & Loretz GmbH...	Aluminium chloride hexahydrate	12323711	2
Caesar & Loretz GmbH	Aluminium chloride hexahydrate	12114906	1
Caesar & Loretz GmbH	Aluminium chloride hexahydrate	12114918	1
Caesar & Loretz GmbH	Aluminium chloride hexahydrate	12323702	1
Caesar/Lorenz	Aluminium chloride hexahydrate	12114918	1
Eurho / Sanacorp	Aluminium chloride hexahydrate	12I27-N01	1
EuRho Pharm	Aluminium chloride hexahydrate	1109025-02	1
EuRho	Aluminium chloride hexahydrate	1106017-01	1
EuRho	Aluminium chloride hexahydrate	1210014-01	1
EuRho	Aluminium chloride hexahydrate	2512I01095	1
EuRho	Aluminium chloride hexahydrate	d024a	1
Euro OTC	Aluminium chloride hexahydrate	1103007-01	1
Euro OTC	Aluminium chloride hexahydrate	1109025-01	1
Euro OTC	Aluminium chloride hexahydrate	1109025-02	1
Euro OTC	Aluminium chloride hexahydrate	120402601	1
Euro OTC	Aluminium chloride hexahydrate	1204026-01	16
Euro OTC	Aluminium chloride hexahydrate	120402602	1
Euro OTC	Aluminium chloride hexahydrate	1204026-02	13
Euro OTC	Aluminium chloride hexahydrate	12100014-02	1
Euro OTC	Aluminium chloride hexahydrate	1210012-01	1
Euro OTC	Aluminium chloride hexahydrate	121001401	2
Euro OTC	Aluminium chloride hexahydrate	1210014-01	18
Euro OTC	Aluminium chloride hexahydrate	121001402	1
Euro OTC	Aluminium chloride hexahydrate	1210014-02	24
Euro OTC	Aluminium chloride hexahydrate	1210014-02-336331909	1
Euro OTC	Aluminium chloride hexahydrate	1213M-01095	1
Euro OTC	Aluminium chloride hexahydrate	1307011	1
Euro OTC	Aluminium chloride hexahydrate	1307011-01	10
Euro OTC	Aluminium chloride hexahydrate	1307011-02	2
Euro OTC	Aluminium chloride hexahydrate	1406021-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Aluminium chloride hexahydrate	1507002-01	1
Euro OTC	Aluminium chloride hexahydrate	2111Q-01095	1
Euro OTC	Aluminium chloride hexahydrate	2207005-01	1
Euro OTC	Aluminium chloride hexahydrate	co31a	1
EUro/AHD	Aluminium chloride hexahydrate	121001401	1
EUro/AHD	Aluminium chloride hexahydrate	1210014-01	1
Euroo/Phoenix	Aluminium chloride hexahydrate	120014-02	1
Euroo/Phoenix	Aluminium chloride hexahydrate	1210014-02	2
Fagron	Aluminium chloride hexahydrate		1
Fagron	Aluminium chloride hexahydrate	105282-0001	1
Fagron	Aluminium chloride hexahydrate	11/23-N06	1
Fagron	Aluminium chloride hexahydrate	11/23-N06B206A	1
Fagron	Aluminium chloride hexahydrate	11G05-N02	1
Fagron	Aluminium chloride hexahydrate	11G05-No2	1
Fagron	Aluminium chloride hexahydrate	11l23-N06	3
Fagron	Aluminium chloride hexahydrate	12/11-No3	1
Fagron	Aluminium chloride hexahydrate	12/27/N01	1
Fagron	Aluminium chloride hexahydrate	12/27-n01	1
Fagron	Aluminium chloride hexahydrate	12/27-N01	5
Fagron	Aluminium chloride hexahydrate	12047512	1
Fagron	Aluminium chloride hexahydrate	1207211095	1
Fagron	Aluminium chloride hexahydrate	12082013D	1
Fagron	Aluminium chloride hexahydrate	12323702	2
Fagron	Aluminium chloride hexahydrate	12323711	1
Fagron	Aluminium chloride hexahydrate	12C07-N01	4
Fagron	Aluminium chloride hexahydrate	12G05-N10	23
Fagron	Aluminium chloride hexahydrate	12i27-N01	1
Fagron	Aluminium chloride hexahydrate	12I27-N01	9
Fagron	Aluminium chloride hexahydrate	12L11-N03	2
Fagron	Aluminium chloride hexahydrate	12l27-N01	2
Fagron	Aluminium chloride hexahydrate	13126-N13	1
Fagron	Aluminium chloride hexahydrate	13D22N09	2
Fagron	Aluminium chloride hexahydrate	13D22-N09	19
Fagron	Aluminium chloride hexahydrate	13d22no9	1
Fagron	Aluminium chloride hexahydrate	13G03-N02	19
Fagron	Aluminium chloride hexahydrate	13I26-N13	2
Fagron	Aluminium chloride hexahydrate	13J31-B06-287615	1
Fagron	Aluminium chloride hexahydrate	17F26-B01-340253	1
Fagron	Aluminium chloride hexahydrate	1910211095	1
Fagron	Aluminium chloride hexahydrate	20122013E	1
Fagron	Aluminium chloride hexahydrate	2013U-01095	1
Fagron	Aluminium chloride hexahydrate	2913U1095	1
Fagron	Aluminium chloride hexahydrate	5213A1095	1
Fagron	Aluminium chloride hexahydrate	8547287	1
Fagron	Aluminium chloride hexahydrate	C012A	1
Fagron	Aluminium chloride hexahydrate	C145A	1
Fagron	Aluminium chloride hexahydrate	C181A	1
Fargon	Aluminium chloride hexahydrate	11/23-N06	1
Faron	Aluminium chloride hexahydrate	13I13-B03-287298	1
Fragon	Aluminium chloride hexahydrate	13D22-N09	1
Gehe	Aluminium chloride hexahydrate	11229917	1
Gehe	Aluminium chloride hexahydrate	120402601	1
Gehe	Aluminium chloride hexahydrate	12047512	1
Gehe	Aluminium chloride hexahydrate	1210014-01	2
Gehe	Aluminium chloride hexahydrate	12114902	1
Gehe	Aluminium chloride hexahydrate	12114908	1
Gehe	Aluminium chloride hexahydrate	12114922	1
Gehe	Aluminium chloride hexahydrate	12323711	2
Gehe	Aluminium chloride hexahydrate	130701102	1
Gehe	Aluminium chloride hexahydrate	1911008-04	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Aluminium chloride hexahydrate	21002588009	1
Gehe	Aluminium chloride hexahydrate	22002438001	1
Gehe	Aluminium chloride hexahydrate	22002438005	1
Gehe	Aluminium chloride hexahydrate	2207005-01	1
Gehe	Aluminium chloride hexahydrate	23C23-B17-227777	1
Honeywell	Aluminium chloride hexahydrate	1210014-02	1
Ichthyol-Gesellschaf…	Aluminium chloride hexahydrate	12114918	1
Krömpke	Aluminium chloride hexahydrate	1204026-01	1
Noweda	Aluminium chloride hexahydrate	1109025-02	1
Noweda	Aluminium chloride hexahydrate	12114910	2
Noweda	Aluminium chloride hexahydrate	191008-04	1
Noweda	Aluminium chloride hexahydrate	21K26-B04-216815	1
Noweda	Aluminium chloride hexahydrate	22002438006	1
NOWEDA	Aluminium chloride hexahydrate	22002438006	1
Noweda	Aluminium chloride hexahydrate	2207005-01	3
Noweda	Aluminium chloride hexahydrate	22K14-B01-225219	1
Phoenix	Aluminium chloride hexahydrate	1210014-01	1
Phoenix	Aluminium chloride hexahydrate	13D22-N09	1
Phoenix	Aluminium chloride hexahydrate	2207005-01	1
Phönix Gotha	Aluminium chloride hexahydrate	1210014-02	1
Phönix	Aluminium chloride hexahydrate	12/27-N01	1
Phönix	Aluminium chloride hexahydrate	1204026-02	1
Phönix	Aluminium chloride hexahydrate	1210014-02	1
Phönix	Aluminium chloride hexahydrate	12L11-N03	1
Phönix	Aluminium chloride hexahydrate	22002438001	1
Phönix	Aluminium chloride hexahydrate	22002438010	1
Phönix	Aluminium chloride hexahydrate	2207005-01	1
Sanacorp	Aluminium chloride hexahydrate	1210014-02	1
Sanacorp	Aluminium chloride hexahydrate	12114920	1
Sanacorp	Aluminium chloride hexahydrate	12323717	1
Sanacorp	Aluminium chloride hexahydrate	12C07-N01	1
Sanacorp	Aluminium chloride hexahydrate	22002438001	1
Sanacorp	Aluminium chloride hexahydrate	22002438010	1
Sanacorp	Aluminium chloride hexahydrate	2207005-01	2
Sanacorp	Aluminium chloride hexahydrate	22G29-B04-220832	1
vdL	Aluminium chloride hexahydrate	2207005-01	1

- 235 533 spectra from 1515 *Apo-Ident* customers from a total of 49 122 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	150	0	201 934
Type C	0	530	4	235 533

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9007 %)	99.2509 % (> 98.6891 %)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26049	26556	14.27	174.75
26059	26556	11.52	182.18
26203	26203	0.00	175.06
26556	26556	0.00	183.76
27019	26203	7.52	179.46
27059	26203	11.19	184.35

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ambroxol hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20742-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ambroxol hydrochloride; Ambroxoli hydrochloridum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Ambroxol hydrochloride	10	18	176

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	64.08	–

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ambroxol hydrochloride	161996	22636	40	20160810*
Caelo	Ambroxol hydrochloride	171582	23344	40	20170607*
Euro OTC	Ambroxol hydrochloride	11110008-01	20742	40	1401146
Euro OTC	Ambroxol hydrochloride	1311032-01	21244	40	20131219
Euro OTC	Ambroxol hydrochloride	1509032	21942	60	20151027*
Euro OTC	Ambroxol hydrochloride	1601008	22298	60	20160119*
Euro OTC	Ambroxol hydrochloride	1602015	22347	60	20160217*
Euro OTC	Ambroxol hydrochloride	1604035	22550	40	20160428*
Fagron	Ambroxol hydrochloride	13I24-N02	21230	40	20131017
Fagron	Ambroxol hydrochloride	19E01-B02-361735	24821	40	20190606

Validation samples

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

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 460 spectra of 10 reference samples from the substance/substance group *Ambroxol hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 502 spectra from a total of 2832 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 760 spectra of 21 reference samples from the substance/substance group *Ambroxol hydrochloride*.

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

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ambroxol hydrochloride	172860	23801	40
Caelo	Ambroxol hydrochloride	190618	24524	40
Caelo	Ambroxol hydrochloride	22000044	26000	40
Caelo	Ambroxol hydrochloride	23000573	26842	40
Caelo	Ambroxol hydrochloride	23003608	27246	40
Caelo	Ambroxol hydrochloride	24001656	27433	40
Euro OTC	Ambroxol hydrochloride	1609002	22800	40
Euro OTC	Ambroxol hydrochloride	1702004	23155	40
Euro OTC	Ambroxol hydrochloride	1711021	23894	40
Euro OTC	Ambroxol hydrochloride	1806009	24155	40
Euro OTC	Ambroxol hydrochloride	1811039	24423	40
Euro OTC	Ambroxol hydrochloride	1904001	24623	40
Euro OTC	Ambroxol hydrochloride	1911002	24969	40
Euro OTC	Ambroxol hydrochloride	2011004	25463	40
Euro OTC	Ambroxol hydrochloride	2201029	25943	40
Euro OTC	Ambroxol hydrochloride	2210020	26440	40
Euro OTC	Ambroxol hydrochloride	2402033	27289	40
Fagron	Ambroxol hydrochloride	23I29-B08-002374	27414	40
Caelo	Ambroxol hydrochloride	22000044	26000SI	10
Caelo	Ambroxol hydrochloride	23000573	26842SI	20
Euro OTC	Ambroxol hydrochloride	2201029	25943SI	10

- 201 324 spectra from a total of 4027 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B*

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

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

- 1554 spectra from 556 *Apo-Ident* customers from 177 batches from the substance/substance group *Ambroxol hydrochloride*.
- Among them are spectra of independent samples from 176 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ambroxol hydrochloride	1702004-01	2
	Ambroxol hydrochloride	211020-01	1
	Ambroxol hydrochloride	21I29-B02-215601	1
	Ambroxol hydrochloride	22000044002	4
	Ambroxol hydrochloride	22000044012	1
	Ambroxol hydrochloride	22000044016	6
	Ambroxol hydrochloride	22000044021	17
	Ambroxol hydrochloride	22000044022	1
	Ambroxol hydrochloride	2201029-03	2
	Ambroxol hydrochloride	2210020-01	18
	Ambroxol hydrochloride	2210020-02	6
	Ambroxol hydrochloride	2210020-03	3
	Ambroxol hydrochloride	22J31-B01-224227	1
	Ambroxol hydrochloride	23000573001	4
	Ambroxol hydrochloride	23000573003	12
	Ambroxol hydrochloride	23003608003	5
	Ambroxol hydrochloride	240203301	1
	Ambroxol hydrochloride	AXLO747202207	1
	Ambroxol hydrochloride	CEPABX001L21	1
AHD/EuRho	Ambroxol hydrochloride	2011004-01	1
AHD	Ambroxol hydrochloride	2201029-03	2
AHD	Ambroxol hydrochloride	2210020-01	2
AHD	Ambroxol hydrochloride	2210020-03	1
AHD	Ambroxol hydrochloride	23003608001	3
AHD	Ambroxol hydrochloride	233608001	1
Alliance Healthcare	Ambroxol hydrochloride	20003999017	1
alliance	Ambroxol hydrochloride	2210020-01	1
Anuh Phama Limited	Ambroxol hydrochloride	2201029-03	1
Anuh Pharma ltd	Ambroxol hydrochloride	2201029-01	1
Anzag	Ambroxol hydrochloride	15G15-B01-316109	1
Anzag	Ambroxol hydrochloride	22000044002	1
Anzag	Ambroxol hydrochloride	2210020-01	4
APO IDENT	Ambroxol hydrochloride	1711021-02	2
APO IDENT	Ambroxol hydrochloride	1806009-01	2
apo-ident	Ambroxol hydrochloride	1806009-01	1
Audor Pharma	Ambroxol hydrochloride	1911002-02	2
Caedo	Ambroxol hydrochloride	192983012	1
Caelo	Ambroxol hydrochloride	1602015-02	1
Caelo	Ambroxol hydrochloride	1609002-01	3
Caelo	Ambroxol hydrochloride	1609002-02	2
Caelo	Ambroxol hydrochloride	16199602	1
Caelo	Ambroxol hydrochloride	16199603	2
Caelo	Ambroxol hydrochloride	16309201	2
Caelo	Ambroxol hydrochloride	17002902	2
Caelo	Ambroxol hydrochloride	17002904	1
Caelo	Ambroxol hydrochloride	17002905	1
Caelo	Ambroxol hydrochloride	1702004-02	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ambroxol hydrochloride	170522AH/16309201	1
Caelo	Ambroxol hydrochloride	171102101	1
Caelo	Ambroxol hydrochloride	1711021-02	4
Caelo	Ambroxol hydrochloride	17158201	3
Caelo	Ambroxol hydrochloride	17158202	6
Caelo	Ambroxol hydrochloride	17158203	2
Caelo	Ambroxol hydrochloride	17158204	2
Caelo	Ambroxol hydrochloride	17286001	8
Caelo	Ambroxol hydrochloride	1801306	1
Caelo	Ambroxol hydrochloride	18013201	11
Caelo	Ambroxol hydrochloride	18013202	2
Caelo	Ambroxol hydrochloride	18013202/P-23041821	1
Caelo	Ambroxol hydrochloride	18013205	11
Caelo	Ambroxol hydrochloride	18013206	1
Caelo	Ambroxol hydrochloride	18013208	4
Caelo	Ambroxol hydrochloride	18013209	1
Caelo	Ambroxol hydrochloride	18013211	24
Caelo	Ambroxol hydrochloride	18013214	1
Caelo	Ambroxol hydrochloride	18013216	1
Caelo	Ambroxol hydrochloride	18013219	7
Caelo	Ambroxol hydrochloride	18013221	1
Caelo	Ambroxol hydrochloride	1806009-01	1
Caelo	Ambroxol hydrochloride	1811039-01	2
Caelo	Ambroxol hydrochloride	1904001-01	4
Caelo	Ambroxol hydrochloride	19061803	14
Caelo	Ambroxol hydrochloride	19061804	26
Caelo	Ambroxol hydrochloride	19061805	1
Caelo	Ambroxol hydrochloride	19061809	17
Caelo	Ambroxol hydrochloride	19061813	4
Caelo	Ambroxol hydrochloride	19061815	29
Caelo	Ambroxol hydrochloride	1911002-01	4
Caelo	Ambroxol hydrochloride	1911002-02	1
Caelo	Ambroxol hydrochloride	192983001	25
Caelo	Ambroxol hydrochloride	192983002	4
Caelo	Ambroxol hydrochloride	192983003	3
Caelo	Ambroxol hydrochloride	192983006	21
Caelo	Ambroxol hydrochloride	192983008	37
Caelo	Ambroxol hydrochloride	192983011	3
Caelo	Ambroxol hydrochloride	192983012	19
Caelo	Ambroxol hydrochloride	20003996011	1
Caelo	Ambroxol hydrochloride	20003998002	4
Caelo	Ambroxol hydrochloride	20003999002	34
Caelo	Ambroxol hydrochloride	20003999003	25
Caelo	Ambroxol hydrochloride	20003999008	3
Caelo	Ambroxol hydrochloride	20003999011	15
Caelo	Ambroxol hydrochloride	20003999014	2
Caelo	Ambroxol hydrochloride	20003999015	3
Caelo	Ambroxol hydrochloride	20003999017	16
Caelo	Ambroxol hydrochloride	2000399915	1
Caelo	Ambroxol hydrochloride	2011004-01	1
Caelo	Ambroxol hydrochloride	2021904	1
Caelo	Ambroxol hydrochloride	2100086001	1
Caelo	Ambroxol hydrochloride	21001184001	3
Caelo	Ambroxol hydrochloride	210518/1	1
Caelo	Ambroxol hydrochloride	22000044001	2
Caelo	Ambroxol hydrochloride	22000044002	12
Caelo	Ambroxol hydrochloride	22000044003	18
Caelo	Ambroxol hydrochloride	220000440116	1
Caelo	Ambroxol hydrochloride	22000044012	1
Caelo	Ambroxol hydrochloride	22000044016	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ambroxol hydrochloride	2200044003	1
Caelo	Ambroxol hydrochloride	2200044016	1
Caelo	Ambroxol hydrochloride	2201029-01	1
Caelo	Ambroxol hydrochloride	23000573003	2
Caelo	Ambroxol hydrochloride	26011902	1
Caelo	Ambroxol hydrochloride	27101707	1
Caelo	Ambroxol hydrochloride	AXL0512201612	1
Caeolo/Gehe	Ambroxol hydrochloride	1702004-02	2
Caesar & Loretz GmbH...	Ambroxol hydrochloride	22000044003	1
Caesar & Loretz GmbH...	Ambroxol hydrochloride	22000044016	1
Caesar & Loretz GmbH...	Ambroxol hydrochloride	20003999011	1
Caesar & Loretz GmbH...	Ambroxol hydrochloride	192983008	1
Caesar & Loretz GmbH/AHD	Ambroxol hydrochloride	20003999002	3
Caesar & Loretz GmbH/G	Ambroxol hydrochloride	19061809	3
Caesar & Loretz GmbH/G	Ambroxol hydrochloride	20003999002	1
Caesar & Loretz GmbH/gehe	Ambroxol hydrochloride	19061804	1
Caesar & Loretz GmbH/Gehe	Ambroxol hydrochloride	19061815	1
Caesar & Loretz GmbH/Gehe	Ambroxol hydrochloride	192983012	2
Caesar & Loretz GmbH/Gehe	Ambroxol hydrochloride	20003999002	5
Caesar & Loretz GmbH/Gehe	Ambroxol hydrochloride	20003999011	1
Caesar & Loretz GmbH/Gehe	Ambroxol hydrochloride	22000044002	1
Caesar & Loretz GmbH...	Ambroxol hydrochloride	20003999017	1
Caesar & Loretz GmbH...	Ambroxol hydrochloride	22000044002	1
Caesar & Loretz GmbH/Kehr	Ambroxol hydrochloride	19061804	1
Caesar & Loretz GmbH/Kehr	Ambroxol hydrochloride	22000044003	1
Caesar & Loretz GmbH...	Ambroxol hydrochloride	20003999002	1
Caesar & Loretz GmbH...	Ambroxol hydrochloride	20003999017	1
Caesar & Loretz GmbH...	Ambroxol hydrochloride	22000044002	1
Caesar & Loretz GmbH...	Ambroxol hydrochloride	19061802	1
Caesar & Loretz GmbH...	Ambroxol hydrochloride	192983008	1
Caesar & Loretz GmbH...	Ambroxol hydrochloride	20003999002	2
Caesar & Loretz GmbH...	Ambroxol hydrochloride	22000044003	1
Caesar & Loretz GmbH...	Ambroxol hydrochloride	20003999015	1
Caesar & Loretz GmbH	Ambroxol hydrochloride	17286001	1
Caesar & Loretz GmbH	Ambroxol hydrochloride	18013205	1
Caesar & Loretz GmbH	Ambroxol hydrochloride	18013211	1
Caesar & Loretz GmbH	Ambroxol hydrochloride	18013219	3
Caesar & Loretz GmbH	Ambroxol hydrochloride	19061803	1
Caesar & Loretz GmbH	Ambroxol hydrochloride	19061804	6
Caesar & Loretz GmbH	Ambroxol hydrochloride	19061805	1
Caesar & Loretz GmbH	Ambroxol hydrochloride	19061809	3
Caesar & Loretz GmbH	Ambroxol hydrochloride	19061815	10
Caesar & Loretz GmbH	Ambroxol hydrochloride	192983001	7
Caesar & Loretz GmbH	Ambroxol hydrochloride	192983002	2
Caesar & Loretz GmbH	Ambroxol hydrochloride	192983003	4
Caesar & Loretz GmbH	Ambroxol hydrochloride	192983006	6
Caesar & Loretz GmbH	Ambroxol hydrochloride	192983008	10
Caesar & Loretz GmbH	Ambroxol hydrochloride	192983010	1
Caesar & Loretz GmbH	Ambroxol hydrochloride	192983011	1
Caesar & Loretz GmbH	Ambroxol hydrochloride	192983012	6
Caesar & Loretz GmbH	Ambroxol hydrochloride	20003998002	5
Caesar & Loretz GmbH	Ambroxol hydrochloride	20003999002	13
Caesar & Loretz GmbH	Ambroxol hydrochloride	20003999003	10
Caesar & Loretz GmbH	Ambroxol hydrochloride	20003999008	3
Caesar & Loretz GmbH	Ambroxol hydrochloride	20003999011	8
Caesar & Loretz GmbH	Ambroxol hydrochloride	20003999014	3
Caesar & Loretz GmbH	Ambroxol hydrochloride	20003999017	11
Caesar & Loretz GmbH	Ambroxol hydrochloride	21001184001	2
Caesar & Loretz GmbH	Ambroxol hydrochloride	22000044002	6
Caesar & Loretz GmbH	Ambroxol hydrochloride	22000044003	10

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Ambroxol hydrochloride	22000044012	1
Caesar & Loretz GmbH	Ambroxol hydrochloride	22000044016	4
Caesar & Loretz GmbH	Ambroxol hydrochloride	22000044021	1
Caesar & Loretz	Ambroxol hydrochloride	19061809	1
Cealo/Gehe	Ambroxol hydrochloride	171158204	1
Cealo/Sanacorp	Ambroxol hydrochloride	22000044003	1
Chem & Pharma	Ambroxol hydrochloride	AXL0361201310	1
Ebert & Jacobi	Ambroxol hydrochloride	1806009-01	1
Ensbona/Eimermacher	Ambroxol hydrochloride	1711021-02	1
E-plus	Ambroxol hydrochloride	1711021-02	1
Eu Rho	Ambroxol hydrochloride	1911002-02	1
Eurho / GEHE	Ambroxol hydrochloride	2011004-01	1
EuRho- Phoenix	Ambroxol hydrochloride	2201029-02	1
EuRho/ Anzag	Ambroxol hydrochloride	220504(2201029-01)	1
EuRho/ NOWEDA	Ambroxol hydrochloride	1806009-01	1
EuRho/ NOWEDA	Ambroxol hydrochloride	1811039-01	1
Eurho/AHD	Ambroxol hydrochloride	2011004-01	1
Eurho/Anzag	Ambroxol hydrochloride	1811039-01	1
EuRho/Fiebig	Ambroxol hydrochloride	1811039-01	1
EuRho/Fiebig	Ambroxol hydrochloride	20212004-01	1
EuRho/Gehe	Ambroxol hydrochloride	1911002-02	1
EuRho/Gehe	Ambroxol hydrochloride	2011004-02	1
Eurho/Noweda	Ambroxol hydrochloride	1911002-02	1
EuRho/ph	Ambroxol hydrochloride	1911002-01	1
Eurho/Phoenix	Ambroxol hydrochloride	190400101	1
EuRho	Ambroxol hydrochloride	1602015-02	2
EuRho	Ambroxol hydrochloride	1711021-02	1
EuRho	Ambroxol hydrochloride	1811039-01	1
EuRho	Ambroxol hydrochloride	1911002-01	1
euRho	Ambroxol hydrochloride	1911002-02	1
EuRho	Ambroxol hydrochloride	1911002-02	1
EuRho	Ambroxol hydrochloride	2011001-01	1
EuRho	Ambroxol hydrochloride	2011004-01	1
EuRho	Ambroxol hydrochloride	2011004-03	1
EuRho	Ambroxol hydrochloride	2201029-01	2
EuRho	Ambroxol hydrochloride	2201029-03	2
Euro OCT/	Ambroxol hydrochloride	1904001-01	1
Euro OTC	Ambroxol hydrochloride	1(1806009-01)	1
Euro OTC	Ambroxol hydrochloride	111039-01	1
Euro OTC	Ambroxol hydrochloride	1311032-01	1
Euro OTC	Ambroxol hydrochloride	1509032-01	1
Euro OTC	Ambroxol hydrochloride	1601015-2	1
Euro OTC	Ambroxol hydrochloride	1602015-02	2
Euro OTC	Ambroxol hydrochloride	160215-02	1
Euro OTC	Ambroxol hydrochloride	1604032-01	1
Euro OTC	Ambroxol hydrochloride	1604035-01	3
Euro OTC	Ambroxol hydrochloride	1604035-02	13
Euro OTC	Ambroxol hydrochloride	1609002-01	15
Euro OTC	Ambroxol hydrochloride	1609002-02	21
Euro OTC	Ambroxol hydrochloride	170192	1
Euro OTC	Ambroxol hydrochloride	170200401	1
Euro OTC	Ambroxol hydrochloride	1702004-01	12
Euro OTC	Ambroxol hydrochloride	170200402	1
Euro OTC	Ambroxol hydrochloride	1702004-02	11
Euro OTC	Ambroxol hydrochloride	171102-01	1
Euro OTC	Ambroxol hydrochloride	171102101	1
Euro OTC	Ambroxol hydrochloride	1711021-01	21
Euro OTC	Ambroxol hydrochloride	1711021-01/P-030518	1
Euro OTC	Ambroxol hydrochloride	1711021-02	29
Euro OTC	Ambroxol hydrochloride	1806009	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Ambroxol hydrochloride	1806009-01	34
Euro OTC	Ambroxol hydrochloride	1806009-1	1
Euro OTC	Ambroxol hydrochloride	181103901	3
Euro OTC	Ambroxol hydrochloride	1811039-01	45
Euro OTC	Ambroxol hydrochloride	190400-01	1
Euro OTC	Ambroxol hydrochloride	1904001	2
Euro OTC	Ambroxol hydrochloride	1904001-0	1
Euro OTC	Ambroxol hydrochloride	190400101	2
Euro OTC	Ambroxol hydrochloride	1904001-01	77
Euro OTC	Ambroxol hydrochloride	19040101	1
Euro OTC	Ambroxol hydrochloride	1904401	1
Euro OTC	Ambroxol hydrochloride	191002-01	1
Euro OTC	Ambroxol hydrochloride	191100-01	1
Euro OTC	Ambroxol hydrochloride	19110002-01	1
Euro OTC	Ambroxol hydrochloride	1911001-01	1
Euro OTC	Ambroxol hydrochloride	1911001-02	1
Euro OTC	Ambroxol hydrochloride	191100201	2
Euro OTC	Ambroxol hydrochloride	1911002-01	45
Euro OTC	Ambroxol hydrochloride	191100202	1
Euro OTC	Ambroxol hydrochloride	1911002-02	41
Euro OTC	Ambroxol hydrochloride	1911002-42	1
Euro OTC	Ambroxol hydrochloride	1911008-04	1
Euro OTC	Ambroxol hydrochloride	191102-02	2
Euro OTC	Ambroxol hydrochloride	1911022-01	1
Euro OTC	Ambroxol hydrochloride	1L2001	1
Euro OTC	Ambroxol hydrochloride	2(1904001-01)	1
Euro OTC	Ambroxol hydrochloride	201100401	2
Euro OTC	Ambroxol hydrochloride	2011004-01	71
Euro OTC	Ambroxol hydrochloride	2011004-02	13
Euro OTC	Ambroxol hydrochloride	2011004-03	10
Euro OTC	Ambroxol hydrochloride	2011004-04	1
Euro OTC	Ambroxol hydrochloride	201104-01	1
Euro OTC	Ambroxol hydrochloride	201104-03	1
Euro OTC	Ambroxol hydrochloride	220102901	1
Euro OTC	Ambroxol hydrochloride	2201029-01	42
Euro OTC	Ambroxol hydrochloride	2201029-02	9
Euro OTC	Ambroxol hydrochloride	2201029-03	7
Euro OTC	Ambroxol hydrochloride	220109-02	1
Euro OTC	Ambroxol hydrochloride	220715(2201029-01)	1
Euro OTC	Ambroxol hydrochloride	2210020-01	6
Euro OTC	Ambroxol hydrochloride	2210020-02	2
Euro OTC	Ambroxol hydrochloride	27061702	1
Euro OTC	Ambroxol hydrochloride	3111805	1
Euro OTC	Ambroxol hydrochloride	811030-01	1
Euro OTC	Ambroxol hydrochloride	axl0492201608	1
Euro OTC	Ambroxol hydrochloride	AXL056201709	1
Euro OTC	Ambroxol hydrochloride	AXL0592201803	2
Euro OTC	Ambroxol hydrochloride	AXL0601201807	1
Euro OTC	Ambroxol hydrochloride	CEPABIX001L21	1
Euro/Noweda	Ambroxol hydrochloride	1509032-01	1
Euro/Noweda	Ambroxol hydrochloride	181103901	1
Euro/Phönix	Ambroxol hydrochloride	1904001-01	1
Euro/Phönix	Ambroxol hydrochloride	2201029-01	2
Euroo/Gehe	Ambroxol hydrochloride	1702004-02	1
EuroTOC	Ambroxol hydrochloride	1602015-01	1
EurRho	Ambroxol hydrochloride	2011004-01	1
Fagron	Ambroxol hydrochloride	12K12-N02	1
Fagron	Ambroxol hydrochloride	1602015-01	1
Fagron	Ambroxol hydrochloride	16G12-B06-326184	1
Fagron	Ambroxol hydrochloride	16G12-B06-333330	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Ambroxol hydrochloride	17K30-B04-352348	1
Fiebig	Ambroxol hydrochloride	1911002-01	2
Gatt-Koller	Ambroxol hydrochloride	180600901	1
Gatt-Koller	Ambroxol hydrochloride	181103901	2
Gehe amax	Ambroxol hydrochloride	1904001-01	1
Gehe	Ambroxol hydrochloride	16199602	1
GEHE	Ambroxol hydrochloride	1702004-02	1
GEHE	Ambroxol hydrochloride	1711021-01	1
Gehe	Ambroxol hydrochloride	18013211	1
GEHE	Ambroxol hydrochloride	1904001-01	3
Gehe	Ambroxol hydrochloride	19061804	2
Gehe	Ambroxol hydrochloride	1911002-01	3
Gehe	Ambroxol hydrochloride	192983001	1
Gehe	Ambroxol hydrochloride	20003999002	1
Gehe	Ambroxol hydrochloride	20003999011	1
Gehe	Ambroxol hydrochloride	2011004	1
Gehe	Ambroxol hydrochloride	2011004-02	3
Gehe	Ambroxol hydrochloride	22000044002	1
Gehe	Ambroxol hydrochloride	22000044020	5
Gehe	Ambroxol hydrochloride	2200044020	1
Gehe	Ambroxol hydrochloride	2201029-01	1
Gehe	Ambroxol hydrochloride	2300057001	1
Gehe	Ambroxol hydrochloride	23000573001	2
Gehe	Ambroxol hydrochloride	23000573002	1
Gehe	Ambroxol hydrochloride	2402033-01	2
Hanse/Sanacorp	Ambroxol hydrochloride	22000044001	1
Jenne	Ambroxol hydrochloride	2210020-01	2
Jenne	Ambroxol hydrochloride	23003608002	2
Kehr	Ambroxol hydrochloride	18013201	1
Midas	Ambroxol hydrochloride	2011004-01	1
Noweda 23.07.2019	Ambroxol hydrochloride	19061804	1
Noweda Taucha	Ambroxol hydrochloride	2011004-03	2
Noweda/ Caesar&Loren...	Ambroxol hydrochloride	192983001	1
Noweda/EuRo	Ambroxol hydrochloride	1609002-02	1
Noweda	Ambroxol hydrochloride	1711021-01	1
Noweda	Ambroxol hydrochloride	17158201	2
Noweda	Ambroxol hydrochloride	19061804	1
Noweda	Ambroxol hydrochloride	1911002-02	1
Noweda	Ambroxol hydrochloride	192983012	1
Noweda	Ambroxol hydrochloride	20003999002	2
Noweda	Ambroxol hydrochloride	20003999011	1
Noweda	Ambroxol hydrochloride	20003999017	1
Noweda	Ambroxol hydrochloride	21001184001	1
Noweda	Ambroxol hydrochloride	22000044016	1
Noweda	Ambroxol hydrochloride	22000044021	1
Noweda	Ambroxol hydrochloride	2210020-02	1
Noweda	Ambroxol hydrochloride	AXL0747202207	1
phoenix /eurho	Ambroxol hydrochloride	1911002-01	1
Phoenix 09.10.2017	Ambroxol hydrochloride	1702004-02	2
Phoenix 21.6.2019, 17,35EUR	Ambroxol hydrochloride	1811039-01	1
Phoenix	Ambroxol hydrochloride	1604035-02	1
Phoenix	Ambroxol hydrochloride	200003999011	1
Phoenix	Ambroxol hydrochloride	20003999017	1
Phoenix	Ambroxol hydrochloride	22000044016	1
Phoenix	Ambroxol hydrochloride	3188	1
Phoenix	Ambroxol hydrochloride	3198	1
PHÖNIX	Ambroxol hydrochloride	1702004-01	1
Phönix	Ambroxol hydrochloride	1904001-01	1
Phönix	Ambroxol hydrochloride	22000044002	1
Phönix	Ambroxol hydrochloride	22000044003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Ambroxol hydrochloride	2210020-02	4
Phönix	Ambroxol hydrochloride	AXL0747202207	1
Sana/Hanse	Ambroxol hydrochloride	23003608002	7
Sanacorp EURO	Ambroxol hydrochloride	1806009-01	1
Sanacorp/EuRho	Ambroxol hydrochloride	1806009-01	3
Sanacorp/EuRho	Ambroxol hydrochloride	1904001-01	1
Sanacorp	Ambroxol hydrochloride	170204-02	1
Sanacorp	Ambroxol hydrochloride	1711021-01	2
Sanacorp	Ambroxol hydrochloride	18013219	2
SANACORP	Ambroxol hydrochloride	1811039-01	2
SANACORP	Ambroxol hydrochloride	19061802	1
Sanacorp	Ambroxol hydrochloride	19061815	5
Sanacorp	Ambroxol hydrochloride	1911002-01	1
Sanacorp	Ambroxol hydrochloride	192983001	2
Sanacorp	Ambroxol hydrochloride	20003999003	1
Sanacorp	Ambroxol hydrochloride	21001184001	1
Sanacorp	Ambroxol hydrochloride	22000044002	1
Sanacorp	Ambroxol hydrochloride	22000044015	1
Sanacorp	Ambroxol hydrochloride	22000044016	1
Sanacorp	Ambroxol hydrochloride	22000044021	3
Sanacorp	Ambroxol hydrochloride	2201029-01	1
Sanacorp	Ambroxol hydrochloride	2201029-02	1
Sanacorp	Ambroxol hydrochloride	2201029-03	1
Sanacorp	Ambroxol hydrochloride	23003608002	3
Sanacorp	Ambroxol hydrochloride	720220007	1
synthetisch	Ambroxol hydrochloride	2201029-01	2
Ven Petro	Ambroxol hydrochloride	1911002-01	1
Ven Petrochem&Pharma…	Ambroxol hydrochloride	18013205	1
Ven Petrochem&Pharma/Gehe	Ambroxol hydrochloride	18013211	2
Ven Petro-Chem	Ambroxol hydrochloride	1806009-01	1

- 234 513 spectra from 1515 *Apo-Ident* customers from a total of 49 089 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	460	0	152 502
Type B	0	760	0	201 324
Type C	0	1542	12	234 513

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6957 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2105 %)
Type C	100.0000 % (> 99.9007 %)	99.2278 % (> 99.0347 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20742	20742	0.00	125.26
21230	21942	10.96	143.97
21244	22550	5.90	133.87
21942	21942	0.00	144.24
22298	22298	0.00	134.21
22347	22347	0.00	131.07
22550	22550	0.00	131.73
22636	22636	0.00	126.61
23344	23344	0.00	130.08
24821	21942	11.06	145.00

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

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Amifampridine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20317-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Amifampridine; Amifampridinum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Amifampridine	6	7	45

Second-stage model

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

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	123.57	–
⋮	⋮	⋮
Sodium citrate	>50	178.69
Heparin sodium	>50	191.30
Capsaicin	>50	241.34
Sucrose	>50	488.81
Levocarnitine	>50	562.85
Oxybutynin hydrochloride	>50	583.57
Alfatradiol	>50	594.71
Prednicarbate	>50	629.63
Quinine hydrochloride dihydrate	>50	656.43
Pyridoxal-5-phosphate	>50	692.14
Tetracaine	>50	802.23
Methoxsalen	>50	927.92
Triclosan	>50	952.34
Ciprofloxacin hydrochloride	>50	1138.74
Cyproterone acetate	>50	1322.58
Norethisterone acetate	>50	1461.75
Amitriptyline hydrochloride	>50	2526.08
Valine	>50	3980.96

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Amifampridine	17251208	24177	40	20171117
Caelo	Amifampridine	19180701	25392	40	2104347

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Amifampridine	13F05-N01	20901	41	20130606
Fagron	Amifampridine	16A22-B04-317264	22321	60	20160204
Fagron	Amifampridine	19K01-F01-366966	25175	40	20191219
Inresa	Amifampridine	33-15-IV-56P2749B	22848	40	20160822

Validation samples

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

Type A All calibration spectra.

- 261 spectra of 6 reference samples from the substance/substance group *Amifampridine*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 701 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 350 spectra of 11 reference samples from the substance/substance group *Amifampridine*.

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

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Amifampridine	22000776004	26308	40
Euro OTC	Amifampridine	2108004	25818	50
Euro OTC	Amifampridine	2201034	25951	40
Fagron	Amifampridine	17J11-B01-340962	23766	40
Fagron	Amifampridine	22A22-B04-219578	26136	40
Fagron	Amifampridine	24G03-B01-001048	27378	40
Inresa	Amifampridine	33-16-I-77P3018	23723	40
Caelo	Amifampridine	22000776004	26308SI	20
Euro OTC	Amifampridine	2108004	25818SI	10
Euro OTC	Amifampridine	2201034	25951SI	10
Fagron	Amifampridine	22A22-B04-219578	26136SI	20

- 201 734 spectra from a total of 4038 batches from further 838 substances. These spectra were

recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 98 spectra from 22 *Apo-Ident* customers from 47 batches from the substance/substance group *Amifampridine*.
- Among them are spectra of independent samples from 45 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Amifampridine	B02-2237706	1
Caelo	Amifampridine	13f05-n01	1
Caelo	Amifampridine	14H11-B06-298447	2
Caelo	Amifampridine	17251206	6
Caelo	Amifampridine	17251207	1
Caelo	Amifampridine	17251209	1
Caelo	Amifampridine	17251210	4
Caelo	Amifampridine	19180702	3
Caelo	Amifampridine	19180703	1
Caelo	Amifampridine	193070001	2
Caelo	Amifampridine	193070002	2
Caelo	Amifampridine	19307001	1
Caelo	Amifampridine	21003139002	2
Caelo	Amifampridine	22000776002	1
Caelo	Amifampridine	22000776003	2
Caelo	Amifampridine	33-15-IV-56P2749	1
Caelo	Amifampridine	33-15IV-56P2749B	1
Caesar & Loretz GmbH...	Amifampridine	21003139002	1
Caesar & Loretz GmbH/Gehe	Amifampridine	22000776002	1
Caesar & Loretz GmbH	Amifampridine	19180702	1
Fagron	Amifampridine	11/14-N03	1
Fagron	Amifampridine	11K07-N02	1
Fagron	Amifampridine	13F07-N07	1
Fagron	Amifampridine	13K14-M01	1
Fagron	Amifampridine	13L12-M03	1
Fagron	Amifampridine	13L12-M06	2
Fagron	Amifampridine	14H11-B06	3
Fagron	Amifampridine	15B20-B02	2
Fagron	Amifampridine	16D05-B01	1
Fagron	Amifampridine	16D05-B01-318216	1
Fagron	Amifampridine	16K15-B03-330546	1
Fagron	Amifampridine	17J11-B01-343013	1
Fagron	Amifampridine	17L19-B02-352347	1
Fagron	Amifampridine	18G04-B14-353053	3
Fagron	Amifampridine	20J13-F01	1
Fagron	Amifampridine	21C17-F01-377439	1
Gehe	Amifampridine	13F07-N07	1
Inresa Arzneimittel GmbH	Amifampridine	33-16-I-77P3018/1307	1
Inresa	Amifampridine	33-15-IV-56P2749	2
Inresa	Amifampridine	33-15-IV-56P2749B	3
Inresa	Amifampridine	33-15-IV-56P2749B/22	3
Inresa	Amifampridine	33-16-I-77P3018	3
Inresa	Amifampridine	33-16-I-77P3018/1307	2
Inresa	Amifampridine	3316I77P301816022018	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Inresa	Amifampridine	508670001	1
inresa	Amifampridine	58010001	1
inresa	Amifampridine	580710001	2
Inresa	Amifampridine	580710001	9
inresa	Amifampridine	58710001	2
inresa	Amifampridine	631350001	1
Inresa	Amifampridine	631350001	3
Inresa	Amifampridine	63150001	1
Phönix	Amifampridine	22000776003	1
Phönix	Amifampridine	23000580001	1
Sanacorp	Amifampridine	17251209	2
Sanacorp	Amifampridine	20L14-F03-376279	1

- 235 969 spectra from 1515 *Apo-Ident* customers from a total of 49 212 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	261	0	152 701
Type B	0	350	0	201 734
Type C	0	98	0	235 969

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7011 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.2857 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 93.8776 %)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20901	25392	9.56	316.39
22321	25392	9.12	316.81
22848	25392	12.28	315.05
24177	25392	6.47	318.61
25175	25392	6.45	317.91
25392	25392	0.00	320.92

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Amiloride hydrochloride dihydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21879-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Amiloride hydrochloride dihydrate; Amiloridi hydrochloridum dihydricum

Special notes

When selecting the *Amiloride hydrochloride dihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Amiloride hydrochloride dihydrate	5	3	9

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	102.26	–

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Amiloride hydrochloride d…	13J08-B04-288620	21879	60	AR-16-FG-008919-01
Fagron	Amiloride hydrochloride d…	13J08-B04-304547	22339	60	20131024
Fagron	Amiloride hydrochloride d…	17F02-B06-335953	23525	40	20170630
Fagron	Amiloride hydrochloride d…	23E30-B10-229440	26985	40	20230624
Fagron	Amiloride hydrochloride d…	23E30-B10-229440	26985SI	20	20230624
Fagron	Amiloride hydrochloride d…	23L12-B13-235070	27168	40	20240123

Validation samples

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

Type A All calibration spectra.

- 260 spectra of 6 reference samples from the substance/substance group *Amiloride hydrochloride dihydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.
- 152 702 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

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

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

- 150 spectra of 5 reference samples from the substance/substance group *Amiloride hydrochloride dihydrate*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Amiloride hydrochloride d…	15C25-B05-325653	22834	40
Fagron	Amiloride hydrochloride d…	16K07-B02-329114	23119	40
Fagron	Amiloride hydrochloride d…	21D20-F01-379327	25904	40
Fagron	Amiloride hydrochloride d…	21D20-F01-379327	25904SI	10
Fagron	Amiloride hydrochloride d…	23L12-B13-235070	27168SI†	20

- 201 934 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 10 spectra from 4 *Apo-Ident* customers from 9 batches from the substance/substance group *Amiloride hydrochloride dihydrate*.
- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Ebert 04.04.2014	Amiloride hydrochloride d…	13J08-B04	1
Fagron	Amiloride hydrochloride d…	17J02-B04	1
Fagron	Amiloride hydrochloride d…	17J02-B04-341175	2
Fagron	Amiloride hydrochloride d…	18C08-B03-353047	1
Fagron	Amiloride hydrochloride d…	18K16-B01-360014	1

continued on the next page

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

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Amiloride hydrochloride d…	20h25-f03-373607	1
Fagron	Amiloride hydrochloride d…	3100/07/15	1
Fagron	Amiloride hydrochloride d…	3100-03-12	1
Fagron	Amiloride hydrochloride d…	3100-07-15	1

- 236 057 spectra from 1515 *Apo-Ident* customers from a total of 49 249 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	150	0	201 934
Type C	0	10	0	236 057

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21879	21879	0.00	142.84
22339	21879	5.38	143.13

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23525	21879	48.91	148.18
26985	21879	28.98	141.52
27168	21879	20.83	142.33

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

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Amitriptyline hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	22844-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Amitriptyline hydrochloride; Amitriptylini hydrochloridum

Special notes

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

no information

Applicable documents

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

Validation method

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

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Amitriptyline hydrochloride	6	3	77

Second-stage model

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

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Doxepin hydrochloride	98.43	–
⋮	⋮	⋮
Cyproterone acetate	>50	72.24
Prednicarbate	>50	124.95
Oxybutynin hydrochloride	>50	127.20
Levocarnitine	>50	191.23
Capsaicin	>50	218.53
Tetracaine	>50	228.57
Sodium citrate	>50	237.42
Valine	>50	323.99
Methoxsalen	>50	351.19
Norethisterone acetate	>50	427.43
Pyridoxal-5-phosphate	>50	442.31
Alfatradiol	>50	467.04
Quinine hydrochloride dihydrate	>50	539.42
Ciprofloxacin hydrochloride	>50	596.95
Heparin sodium	>50	639.33
Triclosan	>50	1736.38
Amifampridine	>50	2330.42
Sucrose	>50	2609.06

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Amitriptyline hydrochloride	16C31-B01-325540	22844	40	20160425
Fagron	Amitriptyline hydrochloride	18A16-B06-348643	24180	40	1909242

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Amitriptyline hydrochloride	21G23-B03-213920	25842	50	20210906
Fagron	Amitriptyline hydrochloride	23C04-B07-227329	26663	30	20230327
Inresa	Amitriptyline hydrochloride	005669/17112016	22845	40	1705099
Inresa	Amitriptyline hydrochloride	005669/06022017	23078	40	20160524

Validation samples

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

Type A All calibration spectra.

- 240 spectra of 6 reference samples from the substance/substance group *Amitriptyline hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 722 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 170 spectra of 6 reference samples from the substance/substance group *Amitriptyline hydrochloride*.

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

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Amitriptyline hydrochloride	17E11-B02-335098	23528	40
Fagron	Amitriptyline hydrochloride	19C08-B02-362280	24689	40
Fagron	Amitriptyline hydrochloride	22F28-B04-222454	26282	40
Fagron	Amitriptyline hydrochloride	21G23-B03-213920	25842SI†	10
Fagron	Amitriptyline hydrochloride	22F28-B04-222454	26282SI	20
Fagron	Amitriptyline hydrochloride	23C04-B07-227329	26663SI†	20

- 201 914 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples

are listed in *Appendix B*.

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

- 239 spectra from 107 *Apo-Ident* customers from 85 batches from the substance/substance group *Amitriptyline hydrochloride*.
- Among them are spectra of independent samples from 75 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Amitriptyline hydrochloride		1
	Amitriptyline hydrochloride	2113440	1
	Amitriptyline hydrochloride	22B10-B04	1
	Amitriptyline hydrochloride	22B10-B04-217981	3
	Amitriptyline hydrochloride	2301192	1
	Amitriptyline hydrochloride	23C04-B07-227328	6
	Amitriptyline hydrochloride	23C04-B07-227329	2
	Amitriptyline hydrochloride	23C04-B07-231756	1
	Amitriptyline hydrochloride	23C04-B07-227329	1
	Amitriptyline hydrochloride	B07-2317506	11
	Amitriptyline hydrochloride	B09-2361602	1
AEP	Amitriptyline hydrochloride	23C04-B07-231756	1
Alliance Healthcare	Amitriptyline hydrochloride	23C04-B07-227329	1
Alliance Healthcare	Amitriptyline hydrochloride	23C04-B07-231756	1
Caelo	Amitriptyline hydrochloride	19C08-b02-368626	1
Caelo	Amitriptyline hydrochloride	22B10B04217981	1
Euro OTC	Amitriptyline hydrochloride		1
Euro OTC	Amitriptyline hydrochloride	1019Q-03993	1
Euro OTC	Amitriptyline hydrochloride	1506024	2
Euro OTC	Amitriptyline hydrochloride	19C08-B02-362280	1
Euro OTC	Amitriptyline hydrochloride	2715E-07209	1
Fagron	Amitriptyline hydrochloride	1(1901746)	1
Fagron	Amitriptyline hydrochloride	12496176	1
Fagron	Amitriptyline hydrochloride	12C29-B03-211252	1
Fagron	Amitriptyline hydrochloride	17E-11-B02-335096	1
Fagron	Amitriptyline hydrochloride	17E11-B02-337699	1
Fagron	Amitriptyline hydrochloride	17E11-B02-340187	3
Fagron	Amitriptyline hydrochloride	18A16-B06	2
Fagron	Amitriptyline hydrochloride	18A16-B06-344853	3
Fagron	Amitriptyline hydrochloride	18A16-B06-348642	4
Fagron	Amitriptyline hydrochloride	18A16-B06-348643	2
Fagron	Amitriptyline hydrochloride	18A16-B06-353064	1
Fagron	Amitriptyline hydrochloride	18A16-B06-353065	2
Fagron	Amitriptyline hydrochloride	18A16-B06_346046	1
Fagron	Amitriptyline hydrochloride	1901746	5
Fagron	Amitriptyline hydrochloride	19c08-802-368627	1
Fagron	Amitriptyline hydrochloride	19c08-802372547	1
Fagron	Amitriptyline hydrochloride	19c08-b02	1
Fagron	Amitriptyline hydrochloride	19c08-B02	1
Fagron	Amitriptyline hydrochloride	19C08-B02	8
Fagron	Amitriptyline hydrochloride	19C08-B02-362279	3
Fagron	Amitriptyline hydrochloride	19C08-B02-362280	4
Fagron	Amitriptyline hydrochloride	19C-08-B02-362280	1
Fagron	Amitriptyline hydrochloride	19C08-B02-362281	4

continued on the next page

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Amitriptyline hydrochloride	19C08-B02-363377	1
Fagron	Amitriptyline hydrochloride	19C08-B02-363378	5
Fagron	Amitriptyline hydrochloride	19C08-B02-365573	1
Fagron	Amitriptyline hydrochloride	19C08-B02-365574	5
Fagron	Amitriptyline hydrochloride	19C08-B02-367679	2
Fagron	Amitriptyline hydrochloride	19C08-B02-3686207	1
Fagron	Amitriptyline hydrochloride	19C08-B02-368627	7
Fagron	Amitriptyline hydrochloride	19C08-B02-370336	6
Fagron	Amitriptyline hydrochloride	19C08-B02-372647	6
Fagron	Amitriptyline hydrochloride	19C08-B02-374309	4
Fagron	Amitriptyline hydrochloride	19C08-B02-370336	1
Fagron	Amitriptyline hydrochloride	2012315	1
Fagron	Amitriptyline hydrochloride	2012436	4
Fagron	Amitriptyline hydrochloride	21C29-803	1
Fagron	Amitriptyline hydrochloride	21C29-B03	4
Fagron	Amitriptyline hydrochloride	21C29-B03-211251	1
Fagron	Amitriptyline hydrochloride	21C29-B03-211252	6
Fagron	Amitriptyline hydrochloride	21G23-B03	2
Fagron	Amitriptyline hydrochloride	21G23-B03-213919	1
Fagron	Amitriptyline hydrochloride	21G23-B03-21392	1
Fagron	Amitriptyline hydrochloride	21G23B03213920	1
Fagron	Amitriptyline hydrochloride	21G23-B03-213920	12
Fagron	Amitriptyline hydrochloride	22810-804-217981	1
Fagron	Amitriptyline hydrochloride	22B10-B04	6
Fagron	Amitriptyline hydrochloride	22B10-B04-2113440	1
Fagron	Amitriptyline hydrochloride	22b10-b04-21791	1
Fagron	Amitriptyline hydrochloride	22B10-B04-217981	24
Fagron	Amitriptyline hydrochloride	22B10-B04-2179891	1
Fagron	Amitriptyline hydrochloride	22B10-B04-218072	3
Fagron	Amitriptyline hydrochloride	22B10-B04-217981	1
Fagron	Amitriptyline hydrochloride	2301192	3
Fagron	Amitriptyline hydrochloride	2-36862007	1
Fagron	Amitriptyline hydrochloride	23C04-B07-227329	1
Fagron	Amitriptyline hydrochloride	B02-3686207	1
Fagron	Amitriptyline hydrochloride	B02-3703306	1
Fagron	Amitriptyline hydrochloride	B03-2112502	2
Fagron	Amitriptyline hydrochloride	B03-2139109	1
Fagron	Amitriptyline hydrochloride	B03-2139200	1
Fagron	Amitriptyline hydrochloride	B03-2139200	1
Fagron	Amitriptyline hydrochloride	Fagron	1
Fischar/Gehe	Amitriptyline hydrochloride	B03-2112502	1
Fragon Gehe	Amitriptyline hydrochloride	22B10-B04-217981	1
Fragon/Sanacorp	Amitriptyline hydrochloride	1901746	1
Gehe Rostock	Amitriptyline hydrochloride	19C08-B02	2
Gehe Rostock	Amitriptyline hydrochloride	22B10-B04-217981	2
GEHE	Amitriptyline hydrochloride	17E11-B02	1
Gehe	Amitriptyline hydrochloride	19C08-B02-368627	1
Gehe	Amitriptyline hydrochloride	21C29-B03-211252	1
Gehe	Amitriptyline hydrochloride	23C04-B07-231756	1
INRESA/INRESA	Amitriptyline hydrochloride		1
Inresa	Amitriptyline hydrochloride	17112016/P-17031721	1
Inresa	Amitriptyline hydrochloride	5945/12102017	1
Inresa	Amitriptyline hydrochloride	5945/13122017	1
jenne	Amitriptyline hydrochloride	23c04-b07-231756	1
Kehr	Amitriptyline hydrochloride	23C04-B07-227329	1
Kehr	Amitriptyline hydrochloride	23C04-Bo7-227329	1
Kehr	Amitriptyline hydrochloride	23C04-B07-227329	1
Noweda	Amitriptyline hydrochloride	22B10-B04-217981	1
SANACORP	Amitriptyline hydrochloride	19C08-B02	1
Sanacorp	Amitriptyline hydrochloride	22b10-b04-217981	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Amitriptyline hydrochloride	23C04-B07-227329	1

- 235 828 spectra from 1515 *Apo-Ident* customers from a total of 49 175 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	240	0	152 722
Type B	0	170	0	201 914
Type C	0	239	0	235 828

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.4706 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 97.4895 %)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22844	24180	10.34	158.86
22845	22845	0.00	152.21
23078	22845	3.81	150.77
24180	24180	0.00	163.32
25842	24180	13.44	166.71
26663	22845	9.95	163.82

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Amlodipine besilate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10005976-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Amlodipine besilate; Amlodipini besilas

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Amlodipine besilate	4	1	1

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	123.28	–

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Amlodipine besilate	21J12-B20-217787	26064	40	2301087
Fagron	Amlodipine besilate	23F02-B01-233301	26980	40	20230705
Fagron	Amlodipine besilate	23K14-B07-233516	27176	40	20231205
Hetero Dru...	Amlodipine besilate	AL22090086	26403	40	20220929
Hetero Dru...	Amlodipine besilate	AL22090086	26403SI	20	20220929

Validation samples

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

Type A All calibration spectra.

- 180 spectra of 5 reference samples from the substance/substance group *Amlodipine besilate*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 782 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

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

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

- 60 spectra of 3 reference samples from the substance/substance group *Amlodipine besilate*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Amlodipine besilate	21L15-B03-220098	26073	40
Fagron	Amlodipine besilate	21J12-B20-217787	26064SI†	10
Fagron	Amlodipine besilate	21L15-B03-220098	26073SI	10

- 202 024 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Amlodipine besilate*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Amlodipine besilate	21L15-B03-220098	1

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

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

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	180	0	152 782
Type B	0	60	0	202 024
Type C	0	1	0	236 066

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26064	26064	0.00	281.22
26403	26064	8.81	279.59
26980	26064	7.33	276.54
27176	26064	5.50	276.69

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ammonium hydrogen carbonate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20166-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ammonium hydrogen carbonate; Ammonii hydrogencarbonas

Special notes

When selecting the *Ammonium hydrogen carbonate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Ammonium hydrogen carbonate	2	1	13

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Aluminium chloride hexahydrate	143.02	–

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ammonium hydrogen carbonate	182108	24268	40	20180926*
Caelo	Ammonium hydrogen carbonate	23002439	27078	31	20230929*

Validation samples

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

Type A All calibration spectra.

- 71 spectra of 2 reference samples from the substance/substance group *Ammonium hydrogen carbonate*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 891 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

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

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

- 70 spectra of 2 reference samples from the substance/substance group *Ammonium hydrogen carbonate*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ammonium hydrogen carbonate	21001324	25811	50
Caelo	Ammonium hydrogen carbonate	23002439	27078SI†	20

- 202 014 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 15 spectra from 11 *Apo-Ident* customers from 13 batches from the substance/substance group *Ammonium hydrogen carbonate*.
- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Ammonium hydrogen carbonate	11145612	2
Caelo	Ammonium hydrogen carbonate	12022308	2
Caelo	Ammonium hydrogen carbonate	12322201	1
Caelo	Ammonium hydrogen carbonate	12322204	1
Caelo	Ammonium hydrogen carbonate	13104601	1
Caelo	Ammonium hydrogen carbonate	13104611	1
Caelo	Ammonium hydrogen carbonate	23011404	1
Caelo	Ammonium hydrogen carbonate	24101202	1

continued on the next page

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

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ammonium hydrogen carbonate	25111308	1
Caelo	Ammonium hydrogen carbonate	3091204	1
Caelo	Ammonium hydrogen carbonate	3712Q-01103	1
Caelo	Ammonium hydrogen carbonate	72715338	1
Caelo	Ammonium hydrogen carbonate	9139402	1

- 236 052 spectra from 1515 *Apo-Ident* customers from a total of 49 245 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	71	0	152 891
Type B	0	50	20	202 014
Type C	0	15	0	236 052

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 91.5493 %)
Type B	100.0000 % (> 99.9912 %)	71.4286 % (> 67.1429 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24268	24268	0.00	202.22
27078	27078	0.00	211.61

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

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Amoxicillin trihydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10006096-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Amoxicillin trihydrate; Amoxicillinum trihydricum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Amoxicillin trihydrate	5	2	2

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	63.40	–

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Amoxicillin trihydrate	2301017	26570	40	20230223*
Euro OTC	Amoxicillin trihydrate	2301052	26571	40	20230228*
Euro OTC	Amoxicillin trihydrate	2305004	26764	40	20230703*
Euro OTC	Amoxicillin trihydrate	2306006	26765	40	20230712*
Fagron	Amoxicillin trihydrate	23F29-F01-384940	27023	40	20230703

Validation samples

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

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Amoxicillin trihydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 762 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 140 spectra of 5 reference samples from the substance/substance group *Amoxicillin trihydrate*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Amoxicillin trihydrate	2304002	26662	40
Gatt-Koller	Amoxicillin trihydrate	23J00336	26624	40
Euro OTC	Amoxicillin trihydrate	2301017	26570SI†	20
Euro OTC	Amoxicillin trihydrate	2301052	26571SI†	20
Gatt-Koller	Amoxicillin trihydrate	23J00336	26624SI	20

- 201 944 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 4 spectra from 4 *Apo-Ident* customers from 2 batches from the substance/substance group *Amoxicillin trihydrate*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Amoxicillin trihydrate	221213182	2
	Amoxicillin trihydrate	2305004-01	2

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

- 236 063 spectra from 1515 *Apo-Ident* customers from a total of 49 256 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	136	4	201 944
Type C	0	4	0	236 063

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	97.1429 % (> 95.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26570	26570	0.00	135.45
26571	26571	0.00	134.35
26764	26764	0.00	134.51
26765	26765	0.00	134.23
27023	26570	12.18	134.95

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Amphotericin B**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20933-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Amphotericin B; Amphotericinum B

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Amphotericin B	6	9	8

Second-stage model

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

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	43.48	18.52
Bacitracin	76.60	16.74
⋮	⋮	⋮
Nystatin	>50	20.95
Cyanocobalamin	>50	26.46
Colistin sulfate	>50	26.65
Riboflavin	>50	47.83
Calcium pantothenate	>50	59.20
Estradiol hemihydrate	>50	62.76
Selenium yeast	>50	63.29
alpha-tocopheryl acetate dry concentrate	>50	65.58
Triamcinolone	>50	72.82
Calcium glycerophosphate	>50	78.15
Methylcobalamin	>50	79.92
Estriol	>50	80.79
Gelatine, white	>50	83.75
Hyoscine hydrobromide	>50	128.71
Carmellose sodium	>50	129.08
SyrSpend® SF Alka	>50	142.16
Tosylchloramide sodium	>50	146.43
SyrSpend® SF pH4 neo (Maize starch)	>50	149.63
Rice starch	>50	186.60
Oxalic acid	>50	240.01
Corn starch	>50	244.43
SyrSpend® SF pH4	>50	298.91
Acacia, dried dispersion	>50	343.80
Wheat starch	>50	363.92
Maltodextrin	>50	365.91
Potato starch	>50	382.10
Fructose	>50	479.71

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Amphotericin B	1305033-02	20933	40	1403224
Euro OTC	Amphotericin B	1512026-01	22813	40	20160121
Euro OTC	Amphotericin B	2008028	25397	40	20200930*
Euro OTC	Amphotericin B	2105013	25761	50	20210826*
Fagron	Amphotericin B	13I16-N02	21338	40	1508271
Fagron	Amphotericin B	13I16-N02	21951	60	20130911
Fagron	Amphotericin B	16L06-B04-333234	23530	40	20170103

Validation samples

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

Type A All calibration spectra.

- 310 spectra of 7 reference samples from the substance/substance group *Amphotericin B*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.
- 152 652 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 420 spectra of 12 reference samples from the substance/substance group *Amphotericin B*.
- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Amphotericin B	1803036	24065	40

continued on the next page

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

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Amphotericin B	1903002	24614	40
Euro OTC	Amphotericin B	2202018	26031	40
Euro OTC	Amphotericin B	2203033	26089	40
Euro OTC	Amphotericin B	2209011	26433	40
Euro OTC	Amphotericin B	2301050	26939	40
Euro OTC	Amphotericin B	2401018	27157	40
Fagron	Amphotericin B	20G16-F06-373576	25715	50
Fagron	Amphotericin B	22C16-B01-227326	26538	40
Euro OTC	Amphotericin B	2202018	26031SI	10
Euro OTC	Amphotericin B	2203033	26089SI	20
Fagron	Amphotericin B	22C16-B01-227326	26538SI	20

- 201 664 spectra from a total of 4036 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 21 spectra from 12 *Apo-Ident* customers from 9 batches from the substance/substance group *Amphotericin B*.
- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Amphotericin B	1305033-03	12
Euro OTC	Amphotericin B	1803036-01	1
Euro OTC	Amphotericin B	1903002-01	2
Fagron	Amphotericin B	16D05-B04	1
Fagron	Amphotericin B	16106-b04-333234	1
Fagron	Amphotericin B	18Job-B02-358370	1
Fagron	Amphotericin B	20C03-F01-371264	1
Fagron	Amphotericin B	20F10-F03-372701	1
Fagron	Amphotericin B	5173	1

- 236 046 spectra from 1515 *Apo-Ident* customers from a total of 49 249 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	310	0	152 652
Type B	0	420	0	201 664
Type C	0	21	0	236 046

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0645 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.5714 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 71.4286 %)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20933	20933	0.00	77.64
21338	21338	0.00	80.77
21951	21338	10.59	82.08
22813	20933	9.11	76.60
23530	20933	13.12	77.26
25397	25397	0.00	78.29
25761	25761	0.00	78.46

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

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Arginine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20391-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Arginine; Argininum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Arginine	8	10	61

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Trometamol	79.41	–

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Arginine	1604003	22514	40	20160425*
Euro OTC	Arginine	1608031	22801	40	20160916*
Euro OTC	Arginine	1702014	23154	40	20170316*
Euro OTC	Arginine	2001001	25092	40	20200122*
Euro OTC	Arginine	2208024	26533	40	20230119*
Euro OTC	Arginine	2208024	26533SI	20	20230119*
Fagron	Arginine	13J28-B02	21226	40	AR-15-FG-008045-01
Fagron	Arginine	16H24-B04-335673	23748	40	20161010
Fagron	Arginine	21L16-B02-220332	26132	40	20220401
Fagron	Arginine	21L16-B02-220332	26132SI	20	20220401

Validation samples

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

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 10 reference samples from the substance/substance group *Arginine*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 602 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 420 spectra of 11 reference samples from the substance/substance group *Arginine*.

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

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Arginine	1710010	23774	40
Euro OTC	Arginine	1806010	24154	40
Euro OTC	Arginine	1902024	24478	40
Euro OTC	Arginine	1909005	24856	40
Euro OTC	Arginine	2008003	25477	40
Euro OTC	Arginine	2107003	25774	50
Euro OTC	Arginine	2203019	26030	40
Euro OTC	Arginine	2307009	26867	40
Euro OTC	Arginine	2402021	27141	40
Fagron	Arginine	24A10-B07-235268	27170	40
Euro OTC	Arginine	2203019	26030SI	10

- 201 664 spectra from a total of 4035 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 119 spectra from 29 *Apo-Ident* customers from 63 batches from the substance/substance group *Arginine*.

- Among them are spectra of independent samples from 61 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Arginine	21L-16-B02-220332	4
	Arginine	22G19-B03-221821	2
Caelo	Arginine	13J28-B02-290463	1
Caelo	Arginine	14124-B08-303720	1
Caelo	Arginine	15C10-B03-314547	1
Caelo	Arginine	15C10-B03-318785	1
Caelo	Arginine	17G10-B07-347888	1
Euro OTC	Arginine	1105040-01	1
Euro OTC	Arginine	1604003-01	1
Euro OTC	Arginine	1710010-01	2
Euro OTC	Arginine	17122746	1
Euro OTC	Arginine	1902024-01	6
Euro OTC	Arginine	1909005-01	5
Euro OTC	Arginine	2001001-01	3
Euro OTC	Arginine	2001001-1	1
Euro OTC	Arginine	2008003-01	2
Euro OTC	Arginine	2009040-01	3
Euro OTC	Arginine	20113317	1
Euro OTC	Arginine	L1206006-01	1
Fagron	Arginine	12C21-N04	1
Fagron	Arginine	13031801	1
Fagron	Arginine	13F14-N02	2
Fagron	Arginine	13J28-B02-290463	6
Fagron	Arginine	14/24-B08-303720	4
Fagron	Arginine	14/24-B08-303721	2
Fagron	Arginine	14/24-B08-303901	1
Fagron	Arginine	14062019	1
Fagron	Arginine	14092035	2
Fagron	Arginine	1424-B08-303720	1
Fagron	Arginine	14B25-B04	2
Fagron	Arginine	14B25-B04-295749	1
Fagron	Arginine	14I24-B08-303901	1
Fagron	Arginine	14I24-B-303720	1
Fagron	Arginine	15102258	1
Fagron	Arginine	15C10-B03-318784	1
Fagron	Arginine	16032361	1
Fagron	Arginine	16D11-B01-322156	1
Fagron	Arginine	16D11-B01-323566	2
Fagron	Arginine	16H24-B04-328914	1
Fagron	Arginine	16H24-B04-331399	1
Fagron	Arginine	16H24-B04-334063	2
Fagron	Arginine	16H24-B04-335673	3
Fagron	Arginine	16H24-B04-335674	8
Fagron	Arginine	16H24-B04-341855	1
Fagron	Arginine	17022585	1
Fagron	Arginine	17G10-B07	1
Fagron	Arginine	17G10-B07-345399	2
Fagron	Arginine	17G10-B07-347888	1
Fagron	Arginine	17G10-B07-349772	3
Fagron	Arginine	17G10-B07-352495	1
Fagron	Arginine	17G10-B07-354908	1
Fagron	Arginine	18072859	1
Fagron	Arginine	18J04-B03-357823	5
Fagron	Arginine	18J04-B03-357824	2
Fagron	Arginine	19G04-B05-363253	1
Fagron	Arginine	19g04-b05-364722	1
Fagron	Arginine	19G04-B05-364722	1
Fagron	Arginine	20A16-F07-368384	2
Fagron	Arginine	20E08-F09-370773	1
Fagron	Arginine	21F14-B11-213620	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Arginine	701743-0006	1
Fagron	Arginine	B05-3647202	1
Fargon	Arginine	121429	1
GEHE	Arginine	17G10-B07-341856	2
Phönix	Arginine	L1302006-01	1

- 235 948 spectra from 1515 *Apo-Ident* customers from a total of 49 196 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	420	0	201 664
Type C	0	119	0	235 948

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.5714 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 94.9580 %)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21226	21226	0.00	168.30
22514	22514	0.00	155.77
22801	22801	0.00	143.97
23154	23154	0.00	149.80
23748	25092	5.99	165.86
25092	25092	0.00	170.16
26132	25092	5.84	169.27
26533	26533	0.00	165.17

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Arginine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20657-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Arginine hydrochloride; Arginini hydrochloridum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Arginine hydrochloride	8	8	25

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	83.16	–

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Arginine hydrochloride	1306023-01	21776	60	AR-15-FG-008412-01
Euro OTC	Arginine hydrochloride	1603033	22512	40	20160425*
Euro OTC	Arginine hydrochloride	1610042	22877	40	20161128*
Euro OTC	Arginine hydrochloride	1904014	24628	40	20190509*
Euro OTC	Arginine hydrochloride	2008024	25338	40	20200909*
Euro OTC	Arginine hydrochloride	2105005	25673	40	20210531*
Euro OTC	Arginine hydrochloride	2206021	26424	40	20221206*
Fagron	Arginine hydrochloride	22B28-B04-220548	26163	40	20220602
Fagron	Arginine hydrochloride	22B28-B04-220548	26163SI	20	20220602

Validation samples

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

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Arginine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 602 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 350 spectra of 10 reference samples from the substance/substance group *Arginine hydrochloride*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Arginine hydrochloride	1711014	23875	40
Euro OTC	Arginine hydrochloride	1809012	24313	40
Euro OTC	Arginine hydrochloride	1909026	24937	40
Euro OTC	Arginine hydrochloride	2004004	25141	40
Euro OTC	Arginine hydrochloride	2011006	25460	40
Euro OTC	Arginine hydrochloride	2201019	25922	40
Euro OTC	Arginine hydrochloride	2402022	27147	40
Fagron	Arginine hydrochloride	24A10-B09-236592	27179	40
Euro OTC	Arginine hydrochloride	2201019	25922SI	10
Euro OTC	Arginine hydrochloride	2402022	27147SI	20

- 201 734 spectra from a total of 4037 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 51 spectra from 11 *Apo-Ident* customers from 26 batches from the substance/substance group *Arginine hydrochloride*.

- Among them are spectra of independent samples from 25 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
EuRho	Arginine hydrochloride	1306023-01	1
Euro OTC	Arginine hydrochloride	1306023-01	1
Euro OTC	Arginine hydrochloride	1603033-01	1
Euro OTC	Arginine hydrochloride	1610042-01	1
Euro OTC	Arginine hydrochloride	1610042-02	1
Euro OTC	Arginine hydrochloride	1711014-01	2
Euro OTC	Arginine hydrochloride	1909026-01	1
Euro OTC	Arginine hydrochloride	2004004-01	2
Euro OTC	Arginine hydrochloride	2008024-01	1
Euro OTC	Arginine hydrochloride	2011006-01	2
Euro OTC	Arginine hydrochloride	21011967	1
Euro OTC	Arginine hydrochloride	2105005-01	8
Euro OTC	Arginine hydrochloride	2105005-02	2
Euro OTC	Arginine hydrochloride	2201019-01	6
Euro OTC	Arginine hydrochloride	2202019-01	1
Euro OTC	Arginine hydrochloride	L1212009-01	3
Euro OTC	Arginine hydrochloride	L1407040-01	1
Euro OTC	Arginine hydrochloride	L1407040-02	3
Euro OTC	Arginine hydrochloride	L1506023-01	3
Fagron	Arginine hydrochloride	12C20-N08	1
Fagron	Arginine hydrochloride	13J28-B03	2
Fagron	Arginine hydrochloride	13J28-B03-287766	1
Fagron	Arginine hydrochloride	13j28-b03-287768	1
Fagron	Arginine hydrochloride	13j28-B03-287768	1
Fagron	Arginine hydrochloride	13J28-B032x	1
Hirundo Products Ver…	Arginine hydrochloride	6412784-152	2
Pure encapsulations	Arginine hydrochloride	50152421	1

- 236 016 spectra from 1515 *Apo-Ident* customers from a total of 49 232 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	350	0	201 734
Type C	0	51	0	236 016

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.2857 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 88.2353 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21776	21776	0.00	179.78
22512	22512	0.00	180.90
22877	22877	0.00	181.93
24628	24628	0.00	182.13
25338	25338	0.00	183.06
25673	25673	0.00	182.01
26163	22877	7.44	181.78
26424	26424	0.00	177.69

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

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ascorbic acid**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20394-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ascorbic acid; Acidum ascorbicum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Ascorbic acid	9	20	145

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Carbomers	105.18	–

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

Calibration samples

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

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

Validation samples

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

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

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

- 152 562 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 860 spectra of 23 reference samples from the substance/substance group *Ascorbic acid*.

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

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

- 201 224 spectra from a total of 4025 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B*

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

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

- 339 spectra from 232 *Apo-Ident* customers from 151 batches from the substance/substance group *Ascorbic acid*.
- Among them are spectra of independent samples from 144 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

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

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

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

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar und Loretz	Ascorbic acid	19026202	1
caleo	Ascorbic acid	16345205	1
Canea Pharma/ Phönix	Ascorbic acid	VC2014	1
Canea Pharma	Ascorbic acid	VC1740	1
canea, gehe	Ascorbic acid	VC1242	2
Canea/Gehe/21.10.19	Ascorbic acid	VC1846	1
Cealo/Gehe	Ascorbic acid	17360301	1
CSPC Weisheng	Ascorbic acid	1211170065	1
EuRho	Ascorbic acid	1710032-01	1
Euro OTC	Ascorbic acid	10071418	1
Euro OTC	Ascorbic acid	11121302	1
Euro OTC	Ascorbic acid	12061408	1
Euro OTC	Ascorbic acid	1607025	1
Euro OTC	Ascorbic acid	17011404	1
Euro OTC	Ascorbic acid	17041406	1
Euro OTC	Ascorbic acid	1710032_01	1
Euro OTC	Ascorbic acid	1710032-01	2
Euro OTC	Ascorbic acid	1901044-01	1
Euro OTC	Ascorbic acid	1909018-01	2
Euro OTC	Ascorbic acid	191101201	1
Euro OTC	Ascorbic acid	200202201	1
Euro OTC	Ascorbic acid	2002022-01	10
Euro OTC	Ascorbic acid	200202202	1
Euro OTC	Ascorbic acid	2002022-02	6
Euro OTC	Ascorbic acid	20020222-02	1
Euro OTC	Ascorbic acid	2002023	1
Euro OTC	Ascorbic acid	2002023_01	1
Euro OTC	Ascorbic acid	2002023-01	3
Euro OTC	Ascorbic acid	28081303	1
Euro OTC	Ascorbic acid	DY0261921072	1
Euro OTC	Ascorbic acid	L1202011-02	1
Euro OTC	Ascorbic acid	L1708004	1
Euro OTC	Ascorbic acid	L60502801	1
Fagron	Ascorbic acid	123456	1
Fagron	Ascorbic acid	16345205	1
Fagron	Ascorbic acid	2002022-01	1
Fagron	Ascorbic acid	20D14-B06-201123	1
Gatt-Koller	Ascorbic acid	18020406	1
Gatt-Koller	Ascorbic acid	1802406	2
Gehe/Canea	Ascorbic acid	VC2012	1
Gehe/Gehe	Ascorbic acid	L1505001	1
Gehe	Ascorbic acid	16345202	1
Gehe	Ascorbic acid	16345205	1
GEHE	Ascorbic acid	16345205	1
GEHE	Ascorbic acid	18127805	1
Gehe	Ascorbic acid	20003806018	1
gehe	Ascorbic acid	23000894001	1
Gehe	Ascorbic acid	23000894001	1
Ge-Hh	Ascorbic acid	192143005	1
Gesundform	Ascorbic acid	L1110704	1
Hanse/Sana	Ascorbic acid	233218001	1
Hänseler	Ascorbic acid		1
Internet	Ascorbic acid	X00162LAML	1
iuhj	Ascorbic acid	ouhoh	1
Kehr	Ascorbic acid	17360301	1
Kehr	Ascorbic acid	22001801006	1
KÖGL	Ascorbic acid	1900900	1
Ningxia	Ascorbic acid	201114-C01-A	1
Ningxia	Ascorbic acid	201115-C01-A	1
Northeast Pharmaceut…	Ascorbic acid	DY02622000007	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

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

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

Validation results

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

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

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

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

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21229	21229	0.00	188.26
21317	21229	5.26	186.35
22672	22672	0.00	191.02
22680	22680	0.00	190.66
22789	22789	0.00	199.11
22918	22918	0.00	196.81
23062	23062	0.00	192.53
23288	23288	0.00	188.26
23293	23293	0.00	188.83
24936	24936	0.00	203.67

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ascorbyl palmitate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21053-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ascorbyl palmitate; Ascorbylis palmitas

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Ascorbyl palmitate	7	5	213

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Estriol	85.47	–

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ascorbyl palmitate	13K04-N01	21053	40	1403226
Fagron	Ascorbyl palmitate	13C06-B40-291206	21665	60	20140306
Fagron	Ascorbyl palmitate	15F01-B99-309774	21851	60	20150615
Fagron	Ascorbyl palmitate	17E18-B06-335527	23520	40	20170606
Fagron	Ascorbyl palmitate	17E18-B06-335527	23520SI	40	20170606
Fagron	Ascorbyl palmitate	19D25-B04-361254	24665	40	20190517
Fagron	Ascorbyl palmitate	20L07-F01-375723	25583	40	20201223
Fagron	Ascorbyl palmitate	20L07-F01-375723	25583SI	40	20201223
Fagron	Ascorbyl palmitate	24I26-B11-004333	27471	40	20241007
Fagron	Ascorbyl palmitate	24I26-B11-004333	27471SI	40	20241007

Validation samples

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

Type A All calibration spectra.

- 440 spectra of 10 reference samples from the substance/substance group *Ascorbyl palmitate*. These samples are listed above in the *calibration samples* section. The reference samples come

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

from 7 different batches.

- 152 522 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 440 spectra of 11 reference samples from the substance/substance group *Ascorbyl palmitate*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ascorbyl palmitate	17H04-B01-338484	23987	40
Fagron	Ascorbyl palmitate	18A10-B03-344364	24098	40
Fagron	Ascorbyl palmitate	21G17-B04-213672	26058	40
Fagron	Ascorbyl palmitate	22F07-B01-222885	26604	40
Fagron	Ascorbyl palmitate	23A09-B04-228316	26605	40
Fagron	Ascorbyl palmitate	17H04-B01-338484	23987SI	40
Fagron	Ascorbyl palmitate	18A10-B03-344364	24098SI	40
Fagron	Ascorbyl palmitate	19D25-B04-361254	24665SI†	40
Fagron	Ascorbyl palmitate	21G17-B04-213672	26058SI	40
Fagron	Ascorbyl palmitate	22F07-B01-222885	26604SI	40
Fagron	Ascorbyl palmitate	23A09-B04-228316	26605SI	40

- 201 644 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 698 spectra from 335 *Apo-Ident* customers from 231 batches from the substance/substance group *Ascorbyl palmitate*.

- Among them are spectra of independent samples from 212 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

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

Supplier	Substance	Batch	Spectra
	Ascorbyl palmitate	18B12-B09-525889	1
	Ascorbyl palmitate	21G17-B04-213672	1
	Ascorbyl palmitate	21L16-B09-217351	1
	Ascorbyl palmitate	21L16-B09-221849	1
	Ascorbyl palmitate	22F07-B01	1
	Ascorbyl palmitate	22F07-B01-222885	10
	Ascorbyl palmitate	23A09-B04-228316	6
	Ascorbyl palmitate	23Ao9-B04-228316	1
18J22-B03-525911	Ascorbyl palmitate	Fagron	1
AHC	Ascorbyl palmitate	23A09-B04-228316	1
AHD	Ascorbyl palmitate	23A09-B04-228316	1
Bionorica Ethics/ Noweda	Ascorbyl palmitate	85532	2
Bionorica Ethics/Noweda	Ascorbyl palmitate	82275	2
Bionorica Ethics	Ascorbyl palmitate	82275	1
Bionorica ethics	Ascorbyl palmitate	85532	2
Bionorica EthicsGmbH...	Ascorbyl palmitate	74736	1
Bionorica/Noweda	Ascorbyl palmitate	77773	2
Bionorica/Noweda	Ascorbyl palmitate	82275	1
Bionorica/Noweda	Ascorbyl palmitate	85532	2
Bionorica	Ascorbyl palmitate	74736	1
Bionorica	Ascorbyl palmitate	74962	1
Bionorica	Ascorbyl palmitate	82275	1
Bionorica	Ascorbyl palmitate	85532	1
Bombastus	Ascorbyl palmitate	525526	1
Caelo	Ascorbyl palmitate	15F01-B99-525121	1
Caelo	Ascorbyl palmitate	16810-B04525199	1
Caelo	Ascorbyl palmitate	16B10-B04324111	1
Caelo	Ascorbyl palmitate	16B10-B04-525199	1
Caelo	Ascorbyl palmitate	16B-B04-525283	1
Caelo	Ascorbyl palmitate	16I30-B03-525489	1
Caelo	Ascorbyl palmitate	16l30-B03-525358	2
Caelo	Ascorbyl palmitate	17E18-B06	1
Caelo	Ascorbyl palmitate	17E18-B06-334914	1
Caelo	Ascorbyl palmitate	17H04-B01-525632	1
Caelo	Ascorbyl palmitate	18A10-B03	1
Caelo	Ascorbyl palmitate	18A10-B03-344364	2
Caelo	Ascorbyl palmitate	18B12-B09-525720	1
Caelo	Ascorbyl palmitate	18B12-B09-525721	1
Caelo	Ascorbyl palmitate	18J22-B03-355582	1
Caelo	Ascorbyl palmitate	19D25-B04-361254	2
Caelo	Ascorbyl palmitate	20I01-F04-52693	1
Caelo	Ascorbyl palmitate	B04-2136007	1
Caelo	Ascorbyl palmitate	K50264890	1
DSM Nutritional GmbH	Ascorbyl palmitate	20L07-F01-526513	1
Euro OTC	Ascorbyl palmitate	16I30-B03	1
Euro OTC	Ascorbyl palmitate	17H04-B0152632	1
Fagrin/Noweda	Ascorbyl palmitate	18B12-B09525720	1
Fagron	Ascorbyl palmitate		7
Fagron	Ascorbyl palmitate	10061708	1
Fagron	Ascorbyl palmitate	137-66-6	2
Fagron	Ascorbyl palmitate	13C06-B40-291206	2
Fagron	Ascorbyl palmitate	14I03-N01	1
Fagron	Ascorbyl palmitate	15F01-B99	3
Fagron	Ascorbyl palmitate	15f01-b99-309774	1
Fagron	Ascorbyl palmitate	15F01-B99-52063	1
Fagron	Ascorbyl palmitate	15F01-B99-525063	1
Fagron	Ascorbyl palmitate	15F01-B99-525121	1
Fagron	Ascorbyl palmitate	15F01-B99-525122	2
Fagron	Ascorbyl palmitate	16/30-B03	1
Fagron	Ascorbyl palmitate	16/30-B03-329375	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Ascorbyl palmitate	16/30-B03-330625	3
Fagron	Ascorbyl palmitate	1630-B03-525489	1
Fagron	Ascorbyl palmitate	16B10-B04-525199	2
Fagron	Ascorbyl palmitate	16B10-B04-525228	1
Fagron	Ascorbyl palmitate	16B10-B04-525283	1
Fagron	Ascorbyl palmitate	16I30-B03	3
Fagron	Ascorbyl palmitate	16I30-B03-326543	1
Fagron	Ascorbyl palmitate	16I30-B03-329375	1
Fagron	Ascorbyl palmitate	16I30-B03-330625	1
Fagron	Ascorbyl palmitate	16I30-B03-332623	5
Fagron	Ascorbyl palmitate	16I30-B03-525358	3
Fagron	Ascorbyl palmitate	16I30-B03-525380	2
Fagron	Ascorbyl palmitate	16I30-B03-525425	1
Fagron	Ascorbyl palmitate	16I30-B03-525426	1
Fagron	Ascorbyl palmitate	16I30-B03-525489	1
Fagron	Ascorbyl palmitate	16L30-B03-332623	1
Fagron	Ascorbyl palmitate	17e18-b06	2
Fagron	Ascorbyl palmitate	17E18-B06	1
Fagron	Ascorbyl palmitate	17e18b06334914	1
Fagron	Ascorbyl palmitate	17E18-B06-334914	2
Fagron	Ascorbyl palmitate	17E18-B06-335527	3
Fagron	Ascorbyl palmitate	17E18-B06-336731	2
Fagron	Ascorbyl palmitate	17E18-B06-525514	1
Fagron	Ascorbyl palmitate	17E18-B06-5255225	1
Fagron	Ascorbyl palmitate	17E18-B06-525524	4
Fagron	Ascorbyl palmitate	17E18-B06-525525	1
Fagron	Ascorbyl palmitate	17E18-B06-525526	2
Fagron	Ascorbyl palmitate	17H04-B01	1
Fagron	Ascorbyl palmitate	17H04B01338484	1
Fagron	Ascorbyl palmitate	17H04-B01-338484	8
Fagron	Ascorbyl palmitate	17H04B01340474	2
Fagron	Ascorbyl palmitate	17H04-B01-340474	3
Fagron	Ascorbyl palmitate	17h04-b01-525632	1
Fagron	Ascorbyl palmitate	17H04-B01-525632	4
Fagron	Ascorbyl palmitate	18812b09348867	1
Fagron	Ascorbyl palmitate	18812-B09-525719	2
Fagron	Ascorbyl palmitate	18812-B09-525720	3
Fagron	Ascorbyl palmitate	18812-B09-525721	1
Fagron	Ascorbyl palmitate	188B12-B09-525721	1
Fagron	Ascorbyl palmitate	18A10_B03_344364	1
Fagron	Ascorbyl palmitate	18A10-B03	1
Fagron	Ascorbyl palmitate	18A10B03344364	1
Fagron	Ascorbyl palmitate	18A10-B03-344364	23
Fagron	Ascorbyl palmitate	18A10-B03-525701	7
Fagron	Ascorbyl palmitate	18A10-B23-525701	1
Fagron	Ascorbyl palmitate	18B12-B09	3
Fagron	Ascorbyl palmitate	18B-12-B09-001	1
Fagron	Ascorbyl palmitate	18B12-B09-348867	14
Fagron	Ascorbyl palmitate	18B12-B09-3488670092	1
Fagron	Ascorbyl palmitate	18B12B09525719	1
Fagron	Ascorbyl palmitate	18B12-B09-525719	9
Fagron	Ascorbyl palmitate	18B12-B09-525720	5
Fagron	Ascorbyl palmitate	18B12-B09-525721	5
Fagron	Ascorbyl palmitate	18b12-B09-525799	1
Fagron	Ascorbyl palmitate	18B12-B09525799	1
Fagron	Ascorbyl palmitate	18B12-B09-525799	4
Fagron	Ascorbyl palmitate	18B12-B09-525820	2
Fagron	Ascorbyl palmitate	18B12-B09-525836	3
Fagron	Ascorbyl palmitate	18B12-B09-525888	2
Fagron	Ascorbyl palmitate	18B12-B09-525889	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Ascorbyl palmitate	18B12-B09-52889	1
Fagron	Ascorbyl palmitate	18B12-B09-528899	1
Fagron	Ascorbyl palmitate	18I22-B03-525911	1
Fagron	Ascorbyl palmitate	18I22-B03-525967	1
Fagron	Ascorbyl palmitate	18J22-B03	9
Fagron	Ascorbyl palmitate	18J22-B03_525967	1
Fagron	Ascorbyl palmitate	18j22-b03-355582	2
Fagron	Ascorbyl palmitate	18J22-B03-355582	6
Fagron	Ascorbyl palmitate	18J22-B03-357638	3
Fagron	Ascorbyl palmitate	18J22-B03-361032	1
Fagron	Ascorbyl palmitate	18J22-B03-525911	1
Fagron	Ascorbyl palmitate	18J22-B03525967	1
Fagron	Ascorbyl palmitate	18J22-B03-525967	5
Fagron	Ascorbyl palmitate	18J22-B03-526006	3
Fagron	Ascorbyl palmitate	18J22-B03-529967	1
Fagron	Ascorbyl palmitate	19/12-F02	1
Fagron	Ascorbyl palmitate	19112-F02-526151	1
Fagron	Ascorbyl palmitate	1912-F02	1
Fagron	Ascorbyl palmitate	19-12F02	1
Fagron	Ascorbyl palmitate	1912-F02364765	1
Fagron	Ascorbyl palmitate	1912-F02-521699	1
Fagron	Ascorbyl palmitate	19D25	1
Fagron	Ascorbyl palmitate	19D25-B04	18
Fagron	Ascorbyl palmitate	19d25b04361254	1
Fagron	Ascorbyl palmitate	19D25-B04-361254	24
Fagron	Ascorbyl palmitate	19D25-B04-361255	1
Fagron	Ascorbyl palmitate	19D25-B04-362604	7
Fagron	Ascorbyl palmitate	19D25-B04-526038	10
Fagron	Ascorbyl palmitate	19D25-B04-526062	8
Fagron	Ascorbyl palmitate	19D25-B04-526080	1
Fagron	Ascorbyl palmitate	19D25-B04-526092	6
Fagron	Ascorbyl palmitate	19D25-Bo4-361254	1
Fagron	Ascorbyl palmitate	19I12-F02	4
Fagron	Ascorbyl palmitate	19I12-F02-364756	1
Fagron	Ascorbyl palmitate	19I12-F02-364765	9
Fagron	Ascorbyl palmitate	19I12F02526151	1
Fagron	Ascorbyl palmitate	19I12-F02-526151	2
Fagron	Ascorbyl palmitate	19I12-F02-526152	4
Fagron	Ascorbyl palmitate	19I12F02526170	1
Fagron	Ascorbyl palmitate	19I12-F02-526199	1
Fagron	Ascorbyl palmitate	19K12-K03	1
Fagron	Ascorbyl palmitate	19l12-F02	1
Fagron	Ascorbyl palmitate	19O25-B04	1
Fagron	Ascorbyl palmitate	20/01-F04-373583	1
Fagron	Ascorbyl palmitate	2001-F04	2
Fagron	Ascorbyl palmitate	20101-F04-33584	1
Fagron	Ascorbyl palmitate	20101-F04-373584	1
Fagron	Ascorbyl palmitate	20101-F04-526393	1
Fagron	Ascorbyl palmitate	20A17F02	2
Fagron	Ascorbyl palmitate	20A17-F02	13
Fagron	Ascorbyl palmitate	20A17-F02-256273	1
Fagron	Ascorbyl palmitate	20A17F02368100	3
Fagron	Ascorbyl palmitate	20A17-F02-368100	20
Fagron	Ascorbyl palmitate	20A17-F02-526247	8
Fagron	Ascorbyl palmitate	20A17-F02-526273	12
Fagron	Ascorbyl palmitate	20A17-F02-526362	2
Fagron	Ascorbyl palmitate	20A17-FO2-526273	1
Fagron	Ascorbyl palmitate	20I01-04	1
Fagron	Ascorbyl palmitate	20I01-F04	7
Fagron	Ascorbyl palmitate	20I01-F04-373583	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Ascorbyl palmitate	20I01-F04-373584	4
Fagron	Ascorbyl palmitate	20I01-F04-526393	5
Fagron	Ascorbyl palmitate	20I0-F04-373584	1
Fagron	Ascorbyl palmitate	20l01-F04	1
Fagron	Ascorbyl palmitate	20l01-F04-373583	1
Fagron	Ascorbyl palmitate	20L07-F01	4
Fagron	Ascorbyl palmitate	20l07-f01-375723	1
Fagron	Ascorbyl palmitate	20L07-F01-375723	9
Fagron	Ascorbyl palmitate	20L07-F01-526454	1
Fagron	Ascorbyl palmitate	20L07-F01-526513	1
Fagron	Ascorbyl palmitate	20LO-F01-375723	1
Fagron	Ascorbyl palmitate	21E10-F02	11
Fagron	Ascorbyl palmitate	21E10-F02-378353	8
Fagron	Ascorbyl palmitate	21E10-F02-526522	5
Fagron	Ascorbyl palmitate	21E10-F02-526523	1
Fagron	Ascorbyl palmitate	21E10-F02-526524	1
Fagron	Ascorbyl palmitate	21E10-FO2-526625	1
Fagron	Ascorbyl palmitate	21E1O-259-0010	1
Fagron	Ascorbyl palmitate	21G17-804	1
Fagron	Ascorbyl palmitate	21G17-B04	5
Fagron	Ascorbyl palmitate	21G17-B04-213672	24
Fagron	Ascorbyl palmitate	21G17-BO4	1
Fagron	Ascorbyl palmitate	21G17-BO4-213672	1
Fagron	Ascorbyl palmitate	21L16B09217351	1
Fagron	Ascorbyl palmitate	21L16-B09-217351	5
Fagron	Ascorbyl palmitate	21L16-B09-221849	4
Fagron	Ascorbyl palmitate	21L16-B09W-217351	1
Fagron	Ascorbyl palmitate	21L16-Bo9-217351	1
Fagron	Ascorbyl palmitate	21L16-BO9-217351	1
Fagron	Ascorbyl palmitate	22F07-B01-22285	1
Fagron	Ascorbyl palmitate	22F07-B01-222885	3
Fagron	Ascorbyl palmitate	23061810	1
Fagron	Ascorbyl palmitate	24C13-B08-235298	1
Fagron	Ascorbyl palmitate	25/10/19Fr	1
Fagron	Ascorbyl palmitate	2OIO1-F04-373584	1
Fagron	Ascorbyl palmitate	2OIOF-F04-373583	1
Fagron	Ascorbyl palmitate	2OL07-F01-375723	1
Fagron	Ascorbyl palmitate	525426	1
Fagron	Ascorbyl palmitate	525489	1
Fagron	Ascorbyl palmitate	525524	1
Fagron	Ascorbyl palmitate	525525	1
Fagron	Ascorbyl palmitate	925749	1
Fagron	Ascorbyl palmitate	A17-F02-368100	1
Fagron	Ascorbyl palmitate	BO4-2136702	1
Fagron	Ascorbyl palmitate	F01-3757203	3
Fagron	Ascorbyl palmitate	F02-3681000	1
Fagron	Ascorbyl palmitate	F02-3783503	3
Fagron	Ascorbyl palmitate	F02-5265203	1
Fagron	Ascorbyl palmitate	F04-3735803	2
Fagron	Ascorbyl palmitate	F04-3735804	2
Fagron	Ascorbyl palmitate	Fagron	1
Fagron	Ascorbyl palmitate	K45532790	2
Fagron	Ascorbyl palmitate	K47747490	1
Fagron	Ascorbyl palmitate	K48951290	1
Fagron	Ascorbyl palmitate	K48951390	2
Fagron	Ascorbyl palmitate	K49421190	6
Fagron	Ascorbyl palmitate	K50642890	4
Fagron	Ascorbyl palmitate	K50642890/19D25-B04	1
Fagron	Ascorbyl palmitate	k51125490	1
Fagron	Ascorbyl palmitate	K51125490	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Ascorbyl palmitate	UQ90606133	1
Fagron	Ascorbyl palmitate	UQ91006215	6
Fangro/4	Ascorbyl palmitate	19I12F02364765	1
Fargon/GEHE	Ascorbyl palmitate	19/12-F02-364765	1
Fargon/Noweda	Ascorbyl palmitate	18J22-B03-355582	1
Fargon/Sanacorp	Ascorbyl palmitate	19D25-B04-361254	1
Fargon	Ascorbyl palmitate	18A10-B03-344364	1
Fargon	Ascorbyl palmitate	19D25-B04-361254	1
Fargon	Ascorbyl palmitate	21E10-F02-526523	2
Fargon	Ascorbyl palmitate	21E10-F02-526625	1
Fiebig	Ascorbyl palmitate	20I01-F04-373584	1
Gehe	Ascorbyl palmitate	18B12-B09-348867	1
Gehe	Ascorbyl palmitate	19I12-F02	1
GEHE	Ascorbyl palmitate	22F07-B01-222885	2
L12	Ascorbyl palmitate	18B12-B09	1
Merck	Ascorbyl palmitate	16130-B03	1
Merck	Ascorbyl palmitate	17E18-B06-334914	1
Merck	Ascorbyl palmitate	18J22-B03-357638	1
Merck	Ascorbyl palmitate	K50642890	1
Noweda / Fargon	Ascorbyl palmitate	20A17-F02-368100	1
Noweda 27.12.2019	Ascorbyl palmitate	19D25-B04-526062	1
Noweda	Ascorbyl palmitate	18J22-B03-525697	1
Noweda	Ascorbyl palmitate	18J22-B03-525943	1
Noweda	Ascorbyl palmitate	19D25-B04-362604	1
Noweda	Ascorbyl palmitate	20A17-F02-368100	1
Noweda	Ascorbyl palmitate	23A09-804-228316	1
Noweda	Ascorbyl palmitate	K50642890	1
Noweda_22.01.2020	Ascorbyl palmitate	19D25-B04-526038	1
PHOENIX 30.06.2014	Ascorbyl palmitate	UQ21206229	1
Phoenix	Ascorbyl palmitate	18B12-B09	2
Phoenix	Ascorbyl palmitate	18J22-B03-357638	1
Phoenix	Ascorbyl palmitate	21L16-B09-221849	1
Phoenix	Ascorbyl palmitate	23A09-B04-228316	1
Phoenix	Ascorbyl palmitate	F04-3735803	1
Phönix/Bionorica	Ascorbyl palmitate	18A10-B03-344364	1
Phönix	Ascorbyl palmitate	17H04-B01-52632	1
Phönix	Ascorbyl palmitate	18812-B09-525720	2
PHÖNIX	Ascorbyl palmitate	18a10-B03-344364	1
Phönix	Ascorbyl palmitate	20l01-F04-373583	1
Phönix	Ascorbyl palmitate	21L16-B09-221849	1
Sanacorp	Ascorbyl palmitate	137-66-6	1
Sanacorp	Ascorbyl palmitate	17H04-B01	1
Sanacorp	Ascorbyl palmitate	18B12-B09	1
Sanacorp	Ascorbyl palmitate	19D25-B04-361254	2
Sanacorp	Ascorbyl palmitate	20I01-F04-526393	2
Sanacorp	Ascorbyl palmitate	21g17-b04-213672	1
Sanacorp	Ascorbyl palmitate	22F07-B01-222885	1

- 235 369 spectra from 1514 *Apo-Ident* customers from a total of 49 029 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ascorbyl palmitate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

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

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	440	0	201 644
Type C	0	689	9	235 369

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6364 %)
Type C	100.0000 % (> 99.9007 %)	98.7106 % (> 98.2808 %)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21053	21053	0.00	87.04
21665	21053	38.94	85.47
21851	21053	43.39	86.72
23520	21053	26.65	87.83
24665	21053	18.58	87.70
25583	21053	36.73	87.70
27471	21053	44.47	87.61

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

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Aspartic acid**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10005413-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Aspartic acid; Acidum asparticum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Aspartic acid	2	1	0

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Glutamic acid	45.81	–
Glycine	84.89	–

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Aspartic acid	2108022	25775	50	20210906*
Euro OTC	Aspartic acid	2402020	27156	30	20240322*
Euro OTC	Aspartic acid	2402020	27156SI	20	20240322*

Validation samples

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

Type A All calibration spectra.

- 100 spectra of 3 reference samples from the substance/substance group *Aspartic acid*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 862 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 60 spectra of 2 reference samples from the substance/substance group *Aspartic acid*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Aspartic acid	2307035	26873	40
Euro OTC	Aspartic acid	2307035	26873SI	20

- 202 024 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

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

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	100	0	152 862
Type B	0	60	0	202 024
Type C	0	0	0	236 067

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25775	25775	0.00	100.97
27156	27156	0.00	132.53

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Atropine sulfate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20653-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Atropine sulfate; Atropine sulphate; Atropini sulfas

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Atropine sulfate	7	6	32

Second-stage model

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

- Submodel 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	79.92	–
⋮	⋮	⋮
Mometasone furoate	>50	43.26
Potassium sorbate	>50	110.83
Propranolol hydrochloride	>50	149.70
Magnesium hydrogen citrate	>50	169.38
Hydrocortisone	>50	239.00
Quinoline yellow	>50	251.76
Saccharin sodium	>50	279.62
Phenytoin	>50	302.00
Escin, water-soluble	>50	436.09
Calcium orotate dihydrate	>50	481.80

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Atropine sulfate	11180602	20653	30	1405538
Caelo	Atropine sulfate	13173808	21088	40	1403483
Caelo	Atropine sulfate	13357405	21551	50	1504594
Caelo	Atropine sulfate	14336806	21719	60	1510209
Caelo	Atropine sulfate	14336806	21719SI	60	1510209
Caelo	Atropine sulfate	15301601	21920	60	20150930
Caelo	Atropine sulfate	15301601	21920SI	60	20150930
Caelo	Atropine sulfate	172732	23682	40	20171020*
Fagron	Atropine sulfate	16G20-B06-328437	22932	40	20160823

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

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

Type A All calibration spectra.

- 440 spectra of 9 reference samples from the substance/substance group *Atropine sulfate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.
- 152 522 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 550 spectra of 14 reference samples from the substance/substance group *Atropine sulfate*.
- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Atropine sulfate	16326802	22952	40
Caelo	Atropine sulfate	170264	23367	40
Caelo	Atropine sulfate	22002311	26353	40
Caelo	Atropine sulfate	23002005	26949	40
Fagron	Atropine sulfate	22E05-B03-220032	26298	40
Fagron	Atropine sulfate	23J24-B05-233615	27241	40
Caelo	Atropine sulfate	16326802	22952SI	40
Caelo	Atropine sulfate	170264	23367SI	40
Caelo	Atropine sulfate	172732	23682SI†	30
Caelo	Atropine sulfate	22002311	26353SI	40
Caelo	Atropine sulfate	23002005	26949SI	40
Fagron	Atropine sulfate	16G20-B06-328437	22932SI†	40
Fagron	Atropine sulfate	22E05-B03-220032	26298SI	40
Fagron	Atropine sulfate	23J24-B05-233615	27241SI	40

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

- 201 534 spectra from a total of 4037 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 87 spectra from 65 *Apo-Ident* customers from 33 batches from the substance/substance group *Atropine sulfate*.
- Among them are spectra of independent samples from 32 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Atropine sulfate	23000208003	7
	Atropine sulfate	23002005004	2
	Atropine sulfate	23J24-B05-233615	1
AHD	Atropine sulfate	23000208003	1
ATS 200005	Atropine sulfate	21000738004	1
Caelo	Atropine sulfate	13173809	1
Caelo	Atropine sulfate	13357403	1
Caelo	Atropine sulfate	13357405	1
Caelo	Atropine sulfate	14336807	1
Caelo	Atropine sulfate	15115201	3
Caelo	Atropine sulfate	16326802	3
Caelo	Atropine sulfate	16c15b03-319166	1
Caelo	Atropine sulfate	17273202	1
Caelo	Atropine sulfate	18099107	1
Caelo	Atropine sulfate	18099111	3
Caelo	Atropine sulfate	18276501	1
Caelo	Atropine sulfate	18276510	2
Caelo	Atropine sulfate	192937003	1
Caelo	Atropine sulfate	192937007	4
Caelo	Atropine sulfate	21000146001	1
Caelo	Atropine sulfate	21000738001	7
Caelo	Atropine sulfate	21000738004	4
Caelo	Atropine sulfate	21000738007	2
Caelo	Atropine sulfate	22000757003	2
Caelo	Atropine sulfate	22002311003	3
Caelo	Atropine sulfate	70446207	1
Caelo	Atropine sulfate	738001	1
Caesar & Loretz GmbH...	Atropine sulfate	18276501	1
Caesar & Loretz GmbH...	Atropine sulfate	192937007	1
Caesar & Loretz GmbH...	Atropine sulfate	21000738004	1
Caesar & Loretz GmbH...	Atropine sulfate	18099111	1
Caesar & Loretz GmbH...	Atropine sulfate	22000757003	1
Caesar & Loretz GmbH...	Atropine sulfate	182765	1
Caesar & Loretz GmbH...	Atropine sulfate	192937	1
Caesar & Loretz GmbH...	Atropine sulfate	192937007	1
Caesar & Loretz GmbH	Atropine sulfate	192937003	2
Caesar & Loretz GmbH	Atropine sulfate	192937007	4
Caesar & Loretz GmbH	Atropine sulfate	21000738001	2
Caesar & Loretz GmbH	Atropine sulfate	22000757003	4
fargon	Atropine sulfate	13K01-N01	1

continued on the next page

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Atropine sulfate	16326802	1
GEHE	Atropine sulfate	17273202	1
Noweda	Atropine sulfate	12250403	1
Noweda	Atropine sulfate	18276510	1
Noweda	Atropine sulfate	23000208002	1
Parthe Apotheke	Atropine sulfate	120/20	1
Parthe Apotheke	Atropine sulfate	50/21	1
Phönix	Atropine sulfate	15301607	1
Sanacorp	Atropine sulfate	23000208003	1

- 235 980 spectra from 1515 *Apo-Ident* customers from a total of 49 225 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	550	0	201 534
Type C	0	84	3	235 980

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.9091 %)
Type C	100.0000 % (> 99.9007 %)	96.5517 % (> 93.1034 %)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20653	20653	0.00	214.92
21088	21088	0.00	202.59
21551	21551	0.00	212.71
21719	21719	0.00	159.45
21920	21719	21.31	178.72
22932	21088	17.92	196.43
23682	23682	0.00	162.86

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Bacitracin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20851-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bacitracin; Bacitracinum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Bacitracin	6	4	102

Second-stage model

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

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	36.39	22.89
Colistin sulfate	59.82	19.45
⋮	⋮	⋮
Cyanocobalamin	>50	55.17
Amphotericin B	>50	55.60
Calcium pantothenate	>50	57.41
Methylcobalamin	>50	71.19
Triamcinolone	>50	72.36
alpha-tocopheryl acetate dry concentrate	>50	73.74
Nystatin	>50	74.11
Estriol	>50	78.92
Gelatine, white	>50	78.94
Estradiol hemihydrate	>50	104.46
Riboflavin	>50	130.60
Selenium yeast	>50	155.60
Calcium glycerophosphate	>50	187.25
Carmellose sodium	>50	213.34
Hyoscine hydrobromide	>50	222.17
SyrSpend® SF Alka	>50	260.96
Tosylchloramide sodium	>50	267.42
Rice starch	>50	344.40
Oxalic acid	>50	364.87
Corn starch	>50	441.99
SyrSpend® SF pH4 neo (Maize starch)	>50	451.03
Acacia, dried dispersion	>50	472.58
SyrSpend® SF pH4	>50	543.47
Maltodextrin	>50	612.74
Wheat starch	>50	644.50
Potato starch	>50	680.90
Fructose	>50	720.57

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Bacitracin	13A-03-N11	20851	40	1401189
Fagron	Bacitracin	14A21-B09-292909	21657	60	1511741
Fagron	Bacitracin	14E23-B03-296243	21686	60	1503715
Fagron	Bacitracin	15C12-B06-309185	21898	60	20150324
Fagron	Bacitracin	15C12-B06-309185	21986	60	9466
Fagron	Bacitracin	16B17-B03-322939	22739	40	20160421
Fagron	Bacitracin	20E-14-F01-373034	25374	40	20200828

Validation samples

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

Type A All calibration spectra.

- 360 spectra of 7 reference samples from the substance/substance group *Bacitracin*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.
- 152 602 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 180 spectra of 5 reference samples from the substance/substance group *Bacitracin*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Bacitracin	16I12-B03-334194	23531	40
Fagron	Bacitracin	17L11-B02-343685	23933	40
Fagron	Bacitracin	18K14-B04-358690	24815	40
Fagron	Bacitracin	23A04-B07-225071	26603	40
Fagron	Bacitracin	23A04-B07-225071	26603SI	20

- 201 904 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 314 spectra from 176 *Apo-Ident* customers from 113 batches from the substance/substance group *Bacitracin*.

- Among them are spectra of independent samples from 102 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Bacitracin	21H03-B04	1
	Bacitracin	21H03-B04-220048	1
	Bacitracin	23A04-B07-225070	4
	Bacitracin	B0722507000	1
18K14-B04-367499	Bacitracin	Fagron	1
AHD	Bacitracin	17L11-B02-344244	1
Bombastus	Bacitracin	17L11-B02-354799	1
Caelo	Bacitracin	14A21-B09-292908	1
Caelo	Bacitracin	14E23-B03-296243	2
Caelo	Bacitracin	15080605	1
Caelo	Bacitracin	15C12-B06-317782	1
Caelo	Bacitracin	16/12-B03	1
Caelo	Bacitracin	16B17-B03	1
Caelo	Bacitracin	16I12-B03-331152	1
Caelo	Bacitracin	17L11-B02-343685	1
Caelo	Bacitracin	17L11-B02-354799	1
Caelo	Bacitracin	17L11-B02-357635	1
Caelo	Bacitracin	C2280092	1
Caelo	Bacitracin	F01-3732508	2
Euro OTC	Bacitracin	17L11-B02-348461	1
fag	Bacitracin	17L11-B02-346531	1
Fagraon	Bacitracin	14E23-B03-303424	1
Fagron	Bacitracin		1
Fagron	Bacitracin	11J17-N01	2
Fagron	Bacitracin	12G12-N17	1
Fagron	Bacitracin	13A03-N11	1
Fagron	Bacitracin	13B25-B01	1
Fagron	Bacitracin	13C13-N10	1
Fagron	Bacitracin	13D26-N08	1
Fagron	Bacitracin	14A21-B09	2
Fagron	Bacitracin	14A21-B09-290643	2
Fagron	Bacitracin	14A21-B09-290645	2
Fagron	Bacitracin	14A21-B09-292908	2
Fagron	Bacitracin	14E23-B03	3
Fagron	Bacitracin	14e23-b03-296243	1
Fagron	Bacitracin	14E23-B03-296243	6
Fagron	Bacitracin	14E23-B03-296245	2
Fagron	Bacitracin	14E23B03303424	1
Fagron	Bacitracin	14E23B03-303424	1
Fagron	Bacitracin	14E23-B03-303424	3
Fagron	Bacitracin	14E23-B03-333424	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Bacitracin	15C12-B06	1
Fagron	Bacitracin	15C12-B06-309185	1
Fagron	Bacitracin	15C12-B06-317782	1
Fagron	Bacitracin	16/12-B03-329401	3
Fagron	Bacitracin	16/12-B03-331152	1
Fagron	Bacitracin	16/12-B03-334052	3
Fagron	Bacitracin	16/12-B03-334701	1
Fagron	Bacitracin	16/12B03335331	1
Fagron	Bacitracin	16/12-B03-335331	1
Fagron	Bacitracin	1612-B033-334052	1
Fagron	Bacitracin	16B17-B03	2
Fagron	Bacitracin	16B17-B03-321315	1
Fagron	Bacitracin	16b17-b03-322891	1
Fagron	Bacitracin	16B17-b03-322891	1
Fagron	Bacitracin	16B17-B03-322891	10
Fagron	Bacitracin	16b17-b03-322939	1
Fagron	Bacitracin	16B17-B03-322939	1
Fagron	Bacitracin	16B17-B03-323876	1
Fagron	Bacitracin	16B17b03325856	1
Fagron	Bacitracin	16B17B03325856	1
Fagron	Bacitracin	16B17-B03-325856	1
Fagron	Bacitracin	16I12-B03	3
Fagron	Bacitracin	16I12-B03-329401	1
Fagron	Bacitracin	16i12-b03-334052	1
Fagron	Bacitracin	16I12-B03-334052	5
Fagron	Bacitracin	16I12-B03-335331	3
Fagron	Bacitracin	17L11-802	1
Fagron	Bacitracin	17L11-B02	9
Fagron	Bacitracin	17L11-B02_357635	1
Fagron	Bacitracin	17L11-B02-343685	14
Fagron	Bacitracin	17L11-B02-343686	1
Fagron	Bacitracin	17L11-B02-346531	3
Fagron	Bacitracin	17L11-B02-346961	2
Fagron	Bacitracin	17L11B02348461	1
Fagron	Bacitracin	17L11-B02-348461	11
Fagron	Bacitracin	17L11-B02-35400	1
Fagron	Bacitracin	17L11-B02-354799	8
Fagron	Bacitracin	17L11B02357635	1
Fagron	Bacitracin	17L11-B02-357635	7
Fagron	Bacitracin	17L11-B02-357980	1
Fagron	Bacitracin	18K14-B04	10
Fagron	Bacitracin	18k14-B04-358690	1
Fagron	Bacitracin	18K14-B04-358690	17
Fagron	Bacitracin	18K14-B04-358692	1
Fagron	Bacitracin	18K14B04363373	1
Fagron	Bacitracin	18K14-B04363373	1
Fagron	Bacitracin	18K14-B04-363373	6
Fagron	Bacitracin	18K14-B04-367499	3
Fagron	Bacitracin	18K14-B04-368113	1
Fagron	Bacitracin	18K14-B0463373	1
Fagron	Bacitracin	18K14-B04-363374	1
Fagron	Bacitracin	20E14-F01	5
Fagron	Bacitracin	20E14-F01-373033	1
Fagron	Bacitracin	20E14-F01-373258	6
Fagron	Bacitracin	20K20-F02-376064	1
Fagron	Bacitracin	211531	1
Fagron	Bacitracin	21H03_B04_220048	1
Fagron	Bacitracin	21H03-804-216119	1
Fagron	Bacitracin	21H03-B04-216119	3
Fagron	Bacitracin	21H03-B04-216120	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Bacitracin	21H03-B04-220048	3
Fagron	Bacitracin	28051509	1
Fagron	Bacitracin	2917M-03314	1
Fagron	Bacitracin	31071503	1
Fagron	Bacitracin	358690	1
Fagron	Bacitracin	B04-3633703	2
Fagron	Bacitracin	B04-3633704	2
Fagron	Bacitracin	B04-3674909	2
Fagron	Bacitracin	B04-3681103	1
Fagron	Bacitracin	C2208111	2
Fagron	Bacitracin	C2280017	3
Fagron	Bacitracin	C2280054	1
Fagron	Bacitracin	C2280065	3
Fagron	Bacitracin	C2280092	3
Fagron	Bacitracin	C2280111	8
Fagron	Bacitracin	C2280138	3
Fagron	Bacitracin	F01-3730303	2
Fagron	Bacitracin	F01-3732508	5
Fargon - Alliance He...	Bacitracin	21H03-B04-216119	1
Fargon/Gehe	Bacitracin	C2280092	1
Fargon/Phönix	Bacitracin	15C12-B06-312975	1
Fargon/Phönix	Bacitracin	18K14-B04	1
Fargon	Bacitracin	16B17-B03-325856	2
fargon	Bacitracin	17L11-B02-357635	1
Fargron	Bacitracin	16/14-b03-334701	1
Fischar/ Now	Bacitracin	18K14-B04-367499	2
Fragon/ Gehe	Bacitracin	17L11-B02	1
Fragon/Phönix	Bacitracin	16/12-B03-329401	1
Gehe	Bacitracin	16/12-B03-331185	1
Gehe	Bacitracin	16B17-B03-322891	1
Gehe	Bacitracin	17L11-B02-343685	1
Gehe	Bacitracin	17L11-B02-346531	1
Gehe	Bacitracin	17L11-B02-348461	1
gehe	Bacitracin	21H03-B04-216120	2
Gehe	Bacitracin	C2280065	1
Geibo/ Fargron	Bacitracin	16B17-B03-322891	1
Geilenkirchen	Bacitracin	16/12-B03-329401	1
Kehr	Bacitracin	16B17-B03-322891	1
Noweda	Bacitracin	17L11-B02-346961	2
Noweda	Bacitracin	17L11-B02-354800	3
Noweda	Bacitracin	18K14-B04-363373	1
Phönix Gotha	Bacitracin	C2280010	1
Phönix	Bacitracin	c2280065	1
Sanacorp	Bacitracin	18K14-B04	1
Sanacorp	Bacitracin	20E14-F01-373258	1
Sanacorp	Bacitracin	21H03-B04-220048	1
Sanacorp	Bacitracin	21h03-b04-220074	1
sanacorp	Bacitracin	2280111	1
Sanacorp	Bacitracin	23A04-B07-225070	1

- 235 753 spectra from 1515 *Apo-Ident* customers from a total of 49 147 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	180	0	201 904
Type C	0	312	2	235 753

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9007 %)	99.3631 % (> 98.4076 %)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20851	20851	0.00	61.20
21657	21657	0.00	64.71
21686	21686	0.00	68.79
21898	21986	12.70	69.78
21986	21986	0.00	67.98
22739	20851	14.92	66.15
25374	21686	21.82	77.09

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

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Baclofen**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	23375-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Baclofen; Baclofenum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Baclofen	6	3	8

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Dithranol	128.74	–

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Baclofen	21D09-F05-377817	25716	50	20210503
Fagron	Baclofen	21K12-B21-221120	26177	40	20211222
Fagron	Baclofen	21K12-B21-221120	26177SI	20	20211222
Fagron	Baclofen	22K19-B06-225423	26463	40	20221201
Fagron	Baclofen	23K24-B02-234668	27046	40	20231129
Fagron	Baclofen	23K24-B02-234668	27046SI	20	20231129
Fagron	Baclofen	24E21-B01-238856	27300	40	20240613
Inresa	Baclofen	206031617/09062017	23376	40	AR-17-FG-018577-01

Validation samples

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

Type A All calibration spectra.

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 672 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 140 spectra of 4 reference samples from the substance/substance group *Baclofen*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Baclofen	18I28-B02-356294	24444	40
Fagron	Baclofen	20J01-F06-374476	25489	40
Fagron	Baclofen	23G19-B03-230417	26912	40
Fagron	Baclofen	23G19-B03-230417	26912SI	20

- 201 944 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

- 37 spectra from 30 *Apo-Ident* customers from 13 batches from the substance/substance group *Baclofen*.
- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Baclofen		1
	Baclofen	1234567890	1
	Baclofen	201062126	1
	Baclofen	201072217	2
	Baclofen	21K12-B21-221120	2
	Baclofen	22K19-B06-225423	6
	Baclofen	23K24-B02-234668	2
Alliance Healthcare	Baclofen	23K24-B02-234668	1
Fagron	Baclofen	202022126	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Baclofen	21D09-F05	3
Fagron	Baclofen	21d09-f05-377817	1
Fagron	Baclofen	21D09-F05377817	1
Fagron	Baclofen	21D09-F05-377817	12
Gehe	Baclofen	23G19-B03-230417	1
Pharmac. works Polph…	Baclofen	201062126	1

- 236 030 spectra from 1515 *Apo-Ident* customers from a total of 49 245 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	290	0	152 672
Type B	0	140	0	201 944
Type C	0	37	0	236 030

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.9310 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 83.7838 %)

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

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

Identity according to identity test using NIR spectroscopy

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23376	23376	0.00	209.82
25716	23376	7.86	217.41
26177	23376	10.09	216.81
26463	23376	16.03	204.59
27046	23376	12.77	216.79
27300	23376	8.01	214.86

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

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Beclometasone dipropionate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21046-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Beclometasone dipropionate; Beclometasoni dipropionas

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Beclometasone dipropionate	6	4	43

Second-stage model

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

- Submodel 15

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Clobetasol propionate	52.96	58.11
⋮	⋮	⋮
Betamethasone dipropionate	>50	33.20

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Beclometasone dipropionate	1203022-03	21634	55	1509281
Euro OTC	Beclometasone dipropionate	1203022-03	21995	60	20120424
Euro OTC	Beclometasone dipropionate	1502032	22989	40	20150327*
Euro OTC	Beclometasone dipropionate	1502032	22989SI	30	20150327*
Euro OTC	Beclometasone dipropionate	1502032	24869	40	20190828*
Fagron	Beclometasone dipropionate	13I05-N03	21046	60	1511689
Fagron	Beclometasone dipropionate	13E02-B40-293328	21554	40	20140508
Fagron	Beclometasone dipropionate	13E02-B40-296353	21977	60	20140508
Fagron	Beclometasone dipropionate	13E02-B40-296353	21977SI	29	20140508
Fagron	Beclometasone dipropionate	20C17-F03-376057	25743	40	20200518
Fagron	Beclometasone dipropionate	20C17-F03-376057	25743SI	32	20200518

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

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

Type A All calibration spectra.

- 486 spectra of 11 reference samples from the substance/substance group *Beclometasone dipropionate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 476 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

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

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

- 359 spectra of 11 reference samples from the substance/substance group *Beclometasone dipropionate*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Beclometasone dipropionate	15F29-B09-314376	23104	40
Fagron	Beclometasone dipropionate	16B16-B03-342082	23930	40
Fagron	Beclometasone dipropionate	19J02-F03-374146	25717	50
Fagron	Beclometasone dipropionate	21K15-B03-230979	27177	40
Euro OTC	Beclometasone dipropionate	1203022-03	21634†	5
Euro OTC	Beclometasone dipropionate	1203022-03	21995SI†	28
Euro OTC	Beclometasone dipropionate	1502032	24869SI†	31
Fagron	Beclometasone dipropionate	15F29-B09-314376	23104SI	20
Fagron	Beclometasone dipropionate	16B16-B03-342082	23930SI	25
Fagron	Beclometasone dipropionate	19J02-F03-374146	25717SI	40
Fagron	Beclometasone dipropionate	21K15-B03-230979	27177SI	40

- 201 725 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

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

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

- 87 spectra from 35 *Apo-Ident* customers from 48 batches from the substance/substance group *Beclometasone dipropionate*.
- Among them are spectra of independent samples from 42 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Beclometasone dipropionate	13E02-B40-293326	1
Caelo	Beclometasone dipropionate	13I05-N03	2
Caelo	Beclometasone dipropionate	18c05b01358707	1
Caelo	Beclometasone dipropionate	21K15-B03-213640	1
Euro OTC	Beclometasone dipropionate	1203022-01	2
Euro OTC	Beclometasone dipropionate	1203022-03	1
Euro OTC	Beclometasone dipropionate	1502032	1
Euro OTC	Beclometasone dipropionate	1502032-01	1
Euro OTC	Beclometasone dipropionate	1502032-02	3
Euro OTC	Beclometasone dipropionate	1502032-03	2
Euro OTC	Beclometasone dipropionate	18041820	1
Euro OTC	Beclometasone dipropionate	C0783111020	1
Fagro/Noweda	Beclometasone dipropionate	14D04-B04-302335	1
Fagron	Beclometasone dipropionate		1
Fagron	Beclometasone dipropionate	11F28-N02	2
Fagron	Beclometasone dipropionate	11L01-N03	1
Fagron	Beclometasone dipropionate	12D12-N03	4
Fagron	Beclometasone dipropionate	12G04-N11	3
Fagron	Beclometasone dipropionate	13/05-N03	1
Fagron	Beclometasone dipropionate	13/05-NO3	1
Fagron	Beclometasone dipropionate	13E02-B40	1
Fagron	Beclometasone dipropionate	13E02-B40-293327	4
Fagron	Beclometasone dipropionate	13E02-B40-293328	2
Fagron	Beclometasone dipropionate	13E02-B40-296353	1
Fagron	Beclometasone dipropionate	13E02-B40-296354	2
Fagron	Beclometasone dipropionate	13I05N03	1
Fagron	Beclometasone dipropionate	13I05-N03	1
Fagron	Beclometasone dipropionate	14D04-B04-302335	1
Fagron	Beclometasone dipropionate	14D04-B04302336	1
Fagron	Beclometasone dipropionate	14D04-B04-302336	3
Fagron	Beclometasone dipropionate	15F29-B09-314376	1
Fagron	Beclometasone dipropionate	16B16-B03-318877	3
Fagron	Beclometasone dipropionate	16B16-B03-322517	2
Fagron	Beclometasone dipropionate	16B16-B03-333670	2
Fagron	Beclometasone dipropionate	16B16-B03-342082	1
Fagron	Beclometasone dipropionate	18C05-B01-347367	3
Fagron	Beclometasone dipropionate	18C05-B01-347369	5
Fagron	Beclometasone dipropionate	18C05-B01-351434	2
Fagron	Beclometasone dipropionate	18C05-B01-358708	1
Fagron	Beclometasone dipropionate	19J02-F03	3
Fagron	Beclometasone dipropionate	19j02f03365514	2
Fagron	Beclometasone dipropionate	19JO2-F03-365513	1
Fagron	Beclometasone dipropionate	21K15-B03-213638	5
Fagron	Beclometasone dipropionate	21k15b03213639	1
Fagron	Beclometasone dipropionate	21K15-B03-226133	1
Fagron	Beclometasone dipropionate	BMD/M/021/19	1
Fagron	Beclometasone dipropionate	C0783/112020	1
Fagron	Beclometasone dipropionate	F03-3741405	2
Fagron	Beclometasone dipropionate	P-26061721/322517	1
fragon	Beclometasone dipropionate	700721-0004	1

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 235 980 spectra from 1515 *Apo-Ident* customers from a total of 49 210 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

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

	False positive	True positive	False negative	True negative
Type A	0	486	0	152 476
Type B	0	359	0	201 725
Type C	0	85	2	235 980

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

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7654 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.3287 %)
Type C	100.0000 % (> 99.9007 %)	97.7011 % (> 94.2529 %)

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

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

Identity according to identity test using NIR spectroscopy

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

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21046	21046	0.00	63.83
21554	21634	5.22	57.29
21634	21634	0.00	57.37
21977	24869	5.05	61.76
21995	24869	6.98	62.26
22989	22989	0.00	60.33
24869	24869	0.00	60.61
25743	24869	5.42	62.30

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

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Benzocaine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20211-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Benzocaine; Benzocainum

Special notes

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

no information

Applicable documents

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

Validation method

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

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

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

Number of independent samples (batches) in calibration and validation

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

Substance/substance group	Type A	Type B	Type C
Benzocaine	9	10	194

Second-stage model

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

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

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

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	175.06	–

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

Calibration samples

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

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Benzocaine	12341904	20843	40	1411055
Caelo	Benzocaine	13213509	21563	60	1706017
Caelo	Benzocaine	20000972	25195	40	20200513*
Caelo	Benzocaine	22002349	26493	40	20221011*
Caelo	Benzocaine	22002349	26493SI	20	20221011*
Euro OTC	Benzocaine	2207016	26346	40	20221013*
Euro OTC	Benzocaine	2207016	26346SI	20	20221013*
Fagron	Benzocaine	12E04-N06	21083	30	20120607
Fagron	Benzocaine	14G02-B01-306980	23569	40	20140723
Fagron	Benzocaine	16D13-B01-342411	23986	40	1807429
Fagron	Benzocaine	19J11-B11-195266	25172	40	20191031

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 410 spectra of 11 reference samples from the substance/substance group *Benzocaine*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 552 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 430 spectra of 11 reference samples from the substance/substance group *Benzocaine*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Benzocaine	161740	22641	40
Caelo	Benzocaine	172174	23628	40
Caelo	Benzocaine	182778	24378	40
Caelo	Benzocaine	190220	24531	40
Caelo	Benzocaine	20002741	25616	40
Caelo	Benzocaine	210001141	25642	40
Caelo	Benzocaine	21003052	25854	50
Caelo	Benzocaine	24000752	27221	40
Fagron	Benzocaine	22A15-B10-220491	26183	40
Fagron	Benzocaine	23H08-B12-239118	27190	40
Fagron	Benzocaine	22A15-B10-220491	26183SI	20

- 201 654 spectra from a total of 4035 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 806 spectra from 418 *Apo-Ident* customers from 209 batches from the substance/substance group *Benzocaine*.

- Among them are spectra of independent samples from 194 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Benzocaine	21003052007	1
	Benzocaine	21J21-B01-216131	1
	Benzocaine	22002349001	10
	Benzocaine	22002349005	3
	Benzocaine	22002349007	1
	Benzocaine	22G25-B01-222567	1
	Benzocaine	22G25-B01-227344	4
	Benzocaine	22H30-B01-231909	1
	Benzocaine	23H08-B12-239118	1
	Benzocaine	B01-2319009	1
	Benzocaine	C0012201014	1
ACM	Benzocaine	KNC1643J15	1
AHD	Benzocaine	16174001	1
Alliance	Benzocaine	22002349001	1
Anzag / Noweda	Benzocaine	1321351	1
Beiersdorf	Benzocaine	15227314	1
Bombastus	Benzocaine	B02-2007200	2
Caelo	Benzocaine		1
Caelo	Benzocaine	1(19022001)	1
Caelo	Benzocaine	10072603	3
Caelo	Benzocaine	11031703	1
Caelo	Benzocaine	11127506	1
Caelo	Benzocaine	11127508	1
Caelo	Benzocaine	1119E-01118	1
Caelo	Benzocaine	12115007	4
Caelo	Benzocaine	12115008	2
Caelo	Benzocaine	12115011	3
Caelo	Benzocaine	12341904	6
Caelo	Benzocaine	12341906	1
Caelo	Benzocaine	13213502	5
Caelo	Benzocaine	13213509	8
Caelo	Benzocaine	13213515	4
Caelo	Benzocaine	13213516	1
Caelo	Benzocaine	13213518	1
Caelo	Benzocaine	13L06-B02	1
Caelo	Benzocaine	13L06-B02-294112	2
Caelo	Benzocaine	14277502	4
Caelo	Benzocaine	1515I-01118	1
Caelo	Benzocaine	15227301	2
Caelo	Benzocaine	15227302	13
Caelo	Benzocaine	15227307	4
Caelo	Benzocaine	15227311	3
Caelo	Benzocaine	15227312	2
Caelo	Benzocaine	15227313	1
Caelo	Benzocaine	15227314	4
Caelo	Benzocaine	15227315	8
Caelo	Benzocaine	15227315I-201016-1	1
Caelo	Benzocaine	15227317	1
Caelo	Benzocaine	15C19-B04-322019	1
Caelo	Benzocaine	15c19-b04-325359	1
Caelo	Benzocaine	16030403	2
Caelo	Benzocaine	16174001	8
Caelo	Benzocaine	16174001I-290517	1
Caelo	Benzocaine	16174005	2
Caelo	Benzocaine	16174007	9
Caelo	Benzocaine	161740075429	1
Caelo	Benzocaine	161740077	1
Caelo	Benzocaine	16174008	1
Caelo	Benzocaine	16174014	16
Caelo	Benzocaine	16174015	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Benzocaine	16174017	6
Caelo	Benzocaine	16174019	12
Caelo	Benzocaine	161740195459	1
Caelo	Benzocaine	16174020	1
Caelo	Benzocaine	16D13-B01_348062	1
Caelo	Benzocaine	16D13-B01-334195	2
Caelo	Benzocaine	16D13-B01-342411	1
Caelo	Benzocaine	16D13-B01-345969	1
Caelo	Benzocaine	16D13-B01-348062	3
Caelo	Benzocaine	18018801	14
Caelo	Benzocaine	18018804	12
Caelo	Benzocaine	18018805	1
Caelo	Benzocaine	18018806	1
Caelo	Benzocaine	18018808	7
Caelo	Benzocaine	18018810	2
Caelo	Benzocaine	18041803	1
Caelo	Benzocaine	18277801	7
Caelo	Benzocaine	18277802	14
Caelo	Benzocaine	18277805	2
Caelo	Benzocaine	18277806	1
Caelo	Benzocaine	18F-B07-190519	1
Caelo	Benzocaine	1902004	1
Caelo	Benzocaine	19022001	10
Caelo	Benzocaine	19022004	11
Caelo	Benzocaine	19022006	3
Caelo	Benzocaine	19031301	1
Caelo	Benzocaine	19210006	1
Caelo	Benzocaine	192710002	2
Caelo	Benzocaine	192710003	23
Caelo	Benzocaine	192710004	3
Caelo	Benzocaine	192710006	21
Caelo	Benzocaine	19271003	1
Caelo	Benzocaine	19271006	1
Caelo	Benzocaine	192829002	1
Caelo	Benzocaine	20000972003	13
Caelo	Benzocaine	20004054001	3
Caelo	Benzocaine	20004055001	17
Caelo	Benzocaine	21000114002	1
Caelo	Benzocaine	21000114004	8
Caelo	Benzocaine	21000114005	9
Caelo	Benzocaine	21000114006	1
Caelo	Benzocaine	21003052004	8
Caelo	Benzocaine	21003052005	1
Caelo	Benzocaine	21003052007	7
Caelo	Benzocaine	2412M-01118	1
Caelo	Benzocaine	3784947	1
Caelo	Benzocaine	5021401	1
Caelo	Benzocaine	6031501	1
Caelo	Benzocaine	718E-01118	1
Caelo	Benzocaine	91062169	1
Caesaer/Jenne	Benzocaine	16174019	1
Caesar & Loretz GmbH...	Benzocaine	18277801	1
Caesar & Loretz GmbH...	Benzocaine	16174019	1
Caesar & Loretz GmbH...	Benzocaine	1927100	1
Caesar & Loretz GmbH...	Benzocaine	20004055001	1
Caesar & Loretz GmbH...	Benzocaine	192710006	3
Caesar & Loretz GmbH...	Benzocaine	192710006	1
Caesar & Loretz GmbH/GEHE	Benzocaine	192710006	1
Caesar & Loretz GmbH...	Benzocaine	18277801	1
Caesar & Loretz GmbH...	Benzocaine	19022001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Ph	Benzocaine	21000114004	2
Caesar & Loretz GmbH…	Benzocaine	21000114005	1
Caesar & Loretz GmbH…	Benzocaine	21003052004	1
Caesar & Loretz GmbH/Sana	Benzocaine	21000114002	2
Caesar & Loretz GmbH…	Benzocaine	192710003	1
Caesar & Loretz GmbH…	Benzocaine	20000972003	2
Caesar & Loretz GmbH…	Benzocaine	505500001	1
Caesar & Loretz GmbH	Benzocaine	18018808	1
Caesar & Loretz GmbH	Benzocaine	18277801	1
Caesar & Loretz GmbH	Benzocaine	18277802	1
Caesar & Loretz GmbH	Benzocaine	18277806	1
Caesar & Loretz GmbH	Benzocaine	19022001	3
Caesar & Loretz GmbH	Benzocaine	19022004	4
Caesar & Loretz GmbH	Benzocaine	19022006	3
Caesar & Loretz GmbH	Benzocaine	192710003	15
CAESAR & LORETZ GMBH	Benzocaine	192710003	2
Caesar & Loretz GmbH	Benzocaine	192710006	4
Caesar & Loretz GmbH	Benzocaine	20000972003	5
Caesar & Loretz GmbH	Benzocaine	20004054001	1
Caesar & Loretz GmbH	Benzocaine	20004055001	12
Caesar & Loretz GmbH	Benzocaine	21000114002	1
Caesar & Loretz GmbH	Benzocaine	21000114004	6
Caesar & Loretz GmbH	Benzocaine	21000114005	2
Caesar & Loretz GmbH	Benzocaine	21003052004	5
Caesar & Loretz GmbH	Benzocaine	21003052007	4
Caesar & Loretz GmbH	Benzocaine	22002349001	1
Caesar & Loretz GmbH	Benzocaine	22002349005	1
Caesar & Loretz Hild…	Benzocaine	192710003	1
Caesar & Loretz Hilden	Benzocaine	18277801	1
Caesar & Loretz/Geil…	Benzocaine	192710003	1
Caesar & Loretz/Geil…	Benzocaine	20004055001	1
Caesar & Loretz/Geil…	Benzocaine	21000114004	1
Caesar Loretz	Benzocaine	192710006	1
Caleo/Phoenix	Benzocaine	20004055001	1
Cealo	Benzocaine	21000114002	1
Changzhou Sunlight P…	Benzocaine	192710003	1
Changzhou/Noweda	Benzocaine	C0011905005	1
Euro OTC	Benzocaine	13L06-B02-297505	1
Euro OTC	Benzocaine	15227313	1
Euro OTC	Benzocaine	15227314	1
Fagrin/Gehe	Benzocaine	15C19-B04	1
Fagron	Benzocaine		1
Fagron	Benzocaine	104210-0001	1
Fagron	Benzocaine	10K02-N01	1
Fagron	Benzocaine	11/22-N03	1
Fagron	Benzocaine	11/22-N3	1
Fagron	Benzocaine	11K08-B40	4
Fagron	Benzocaine	11K08-B40-291840	1
Fagron	Benzocaine	11k08-b40-291841	1
Fagron	Benzocaine	11k08-B40-291841	1
Fagron	Benzocaine	11K08-B40-291841	6
Fagron	Benzocaine	12341904	1
Fagron	Benzocaine	12E014-N06	1
Fagron	Benzocaine	12E04-N06	9
Fagron	Benzocaine	12H10-N06	3
Fagron	Benzocaine	13F06N10	1
Fagron	Benzocaine	13F06-N10	1
Fagron	Benzocaine	13L06-B02	4
Fagron	Benzocaine	13L06-B02_297505	1
Fagron	Benzocaine	13L06-B02-294100	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Benzocaine	13L06-B02-294112	4
Fagron	Benzocaine	13L06-B02-300480	2
Fagron	Benzocaine	13l06-B02-300494	1
Fagron	Benzocaine	13L06-B02-300494	5
Fagron	Benzocaine	13L06Bo2	1
Fagron	Benzocaine	14G02-B01-306980	1
Fagron	Benzocaine	14G02-B01-310324	8
Fagron	Benzocaine	14G02B01318318	1
Fagron	Benzocaine	14G02-B01-318318	3
Fagron	Benzocaine	15227307	1
Fagron	Benzocaine	15C19-B04	1
Fagron	Benzocaine	15C19-B04-308254	1
Fagron	Benzocaine	15C19-B04-316239	3
Fagron	Benzocaine	15C19-B04-322019	7
Fagron	Benzocaine	15c19-b04-325359	1
Fagron	Benzocaine	15C19-B04-325359	3
Fagron	Benzocaine	15C-19-B04-325359	1
Fagron	Benzocaine	16D113-B01-345969	1
Fagron	Benzocaine	16D13	1
Fagron	Benzocaine	16D13_B01_348062	1
Fagron	Benzocaine	16D13-B01	2
Fagron	Benzocaine	16D13B01330168	1
Fagron	Benzocaine	16D13-B01-330168	1
Fagron	Benzocaine	16D13-b01-334195	1
Fagron	Benzocaine	16D13-B01-334195	3
Fagron	Benzocaine	16D13-B01-337264	4
Fagron	Benzocaine	16D13B01341861	2
Fagron	Benzocaine	16D13-B01-341861	2
Fagron	Benzocaine	16d13-b01-342411	1
Fagron	Benzocaine	16D13-B01-342411	5
Fagron	Benzocaine	16D13B01345969	1
Fagron	Benzocaine	16D13-B01-345969	2
Fagron	Benzocaine	16D13-B01-348062	4
Fagron	Benzocaine	18F18-B50	2
Fagron	Benzocaine	18F18B50352167	1
Fagron	Benzocaine	18F18-B50-352167	2
Fagron	Benzocaine	18F18B50352171	1
Fagron	Benzocaine	18F18-B50-352171	6
Fagron	Benzocaine	18F18B50-353577	1
Fagron	Benzocaine	18F18-B50-353577	6
Fagron	Benzocaine	18F18-B50-35377	1
Fagron	Benzocaine	18F18B50355282	1
Fagron	Benzocaine	18F29-B07	1
Fagron	Benzocaine	18F29-B07_190519	1
Fagron	Benzocaine	18f29b07190519	1
Fagron	Benzocaine	18F29B07190519	1
Fagron	Benzocaine	18F29-B07-190519	19
Fagron	Benzocaine	18F-B50	1
Fagron	Benzocaine	18J31-B02	2
Fagron	Benzocaine	18J31-B02-193431	10
Fagron	Benzocaine	18J31-BO2	1
Fagron	Benzocaine	19G02-B04	1
Fagron	Benzocaine	19J11-011-195266	1
Fagron	Benzocaine	19J11-B11	1
Fagron	Benzocaine	19J11-B11-195266	8
Fagron	Benzocaine	19J11-B11-2000500	1
Fagron	Benzocaine	19J11-B11-200500	5
Fagron	Benzocaine	202522/1	1
Fagron	Benzocaine	20817-801-201337	1
Fagron	Benzocaine	20B17B01201337	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Benzocaine	20B17-B01-201337	1
Fagron	Benzocaine	20C09-B02	2
Fagron	Benzocaine	20C09-B02-200720	8
Fagron	Benzocaine	20C09B02-2007200	1
Fagron	Benzocaine	20G27-B05-201740	1
Fagron	Benzocaine	21A26-B18	1
Fagron	Benzocaine	21A26-B18-204192	2
Fagron	Benzocaine	21D13-B03-210845	3
Fagron	Benzocaine	21G17-B07-214449	1
Fagron	Benzocaine	21J21-B01	1
Fagron	Benzocaine	21J21-B01-216131	1
Fagron	Benzocaine	21J21-B01-218075	3
Fagron	Benzocaine	21J21-BO1-216131	1
Fagron	Benzocaine	22G25-B01-222567	1
Fagron	Benzocaine	2OG27-BO5-201740	1
Fagron	Benzocaine	400313	1
Fagron	Benzocaine	4413E-01118	1
Fagron	Benzocaine	581015	2
Fagron	Benzocaine	B01-2005307	1
Fagron	Benzocaine	B02-2007200	2
Fagron	Benzocaine	B071905109	1
Fagron	Benzocaine	B11-1952606	1
Fagron	Benzocaine	B11-2005000	1
Fagron	Benzocaine	BZ-08/11-12	1
Fagron	Benzocaine	BZ-27/1112	1
Fagron	Benzocaine	C0011803001	1
Fagron	Benzocaine	C0011911003	1
Fagron	Benzocaine	C0012106001	3
Fargon/Sana	Benzocaine	11K08-290049	1
Fargon/Sanacorp	Benzocaine	20C09-B02_200720	1
Fargon	Benzocaine	12H10-N06	1
Fargron	Benzocaine	13L06-B02-294112	1
Fiebig	Benzocaine	13L06-B02-300494	1
Fiebig	Benzocaine	15C19-B04-325359	1
Fiebig	Benzocaine	18018801	1
Fragon	Benzocaine	B02-2007200	1
Gehe	Benzocaine	111214	1
Gehe	Benzocaine	15C19-B04	1
Gehe	Benzocaine	16D13-B01-337264	1
Gehe	Benzocaine	18018801	1
Gehe	Benzocaine	18018808	1
Gehe	Benzocaine	18277801	1
Gehe	Benzocaine	18J31-B02-193431	1
Gehe	Benzocaine	20004055001	1
Gehe	Benzocaine	22002349005	1
Gehe	Benzocaine	22G25-B01-227344	1
Geibo	Benzocaine	22G25-B01-227344	1
Jenne / Fargon	Benzocaine	16D13-B01-337264	1
Jenne	Benzocaine	21003052004	1
Kehr	Benzocaine	15C19-B04-325359	1
Kehr	Benzocaine	16D13-B01-330168	1
L12	Benzocaine	16D13-B01-348062	1
Mömerzheim	Benzocaine	18018804	2
Noweda	Benzocaine	15227313	1
Noweda	Benzocaine	18018804	1
Noweda	Benzocaine	192710003	2
Noweda	Benzocaine	20000972003	1
Noweda	Benzocaine	21000114005	1
Noweda	Benzocaine	22002349007	1
otto geilenkirchen	Benzocaine	192710006	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Benzocaine	12H10-N06	1
Phoenix	Benzocaine	19022001	2
Phoenix	Benzocaine	19022006	1
Phoenix	Benzocaine	192710006	1
Phönix	Benzocaine	13F06-N10	1
Phönix	Benzocaine	20004055001	1
s.Prüfprotokoll	Benzocaine		1
Sanacorp W.E:07.01.1...	Benzocaine	13213502	1
Sanacorp	Benzocaine	13213502	1
Sanacorp	Benzocaine	13213506	1
Sanacorp	Benzocaine	18018801	1

- 235 261 spectra from 1515 *Apo-Ident* customers from a total of 49 053 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Benzocaine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Benzocaine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	410	0	152 552
Type B	0	430	0	201 654
Type C	0	803	3	235 261

The substance/substance group *Benzocaine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5366 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6047 %)
Type C	100.0000 % (> 99.9007 %)	99.6278 % (> 99.2556 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20843	20843	0.00	286.62
21083	21563	56.62	270.56
21563	21563	0.00	283.55
23569	23986	6.59	286.02
23986	23986	0.00	285.82
25172	21563	11.32	283.80
25195	25195	0.00	285.01
26346	26346	0.00	280.75
26493	26493	0.00	280.47

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Benzoic acid**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20041-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Benzoic acid; Acidum benzoicum

Special notes

When selecting the *Benzoic acid* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Benzoic acid	4	2	30

Second-stage model

For differentiation of the substance/substance group *Benzoic acid* the following second-stage model is used:

- Submodel 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Benzoic acid* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Dithranol	73.11	13.34
⋮	⋮	⋮
Sodium salicylate	>50	33.73
Dequalinium chloride	>50	54.06
Acetylsalicylic acid	>50	62.25
Eosin Y	>50	220.87
Oxytetracycline hydrochloride	>50	328.66
Levothyroxin sodium	>50	661.20
Tannin	>50	1493.00

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Benzoic acid* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Benzoic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Benzoic acid	13391310	21458	60	20131216
Caelo	Benzoic acid	15084614	22664	40	20150318
Caelo	Benzoic acid	15084611	23095	40	20150318
Caelo	Benzoic acid	15084614	23096	40	1707644
Caelo	Benzoic acid	15084614	23726	40	20150318
Caelo	Benzoic acid	23001052	26693	40	20230601*
Caelo	Benzoic acid	23001052	26693SI	20	20230601*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 7 reference samples from the substance/substance group *Benzoic acid*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 152 682 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Benzoic acid*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Benzoic acid	162701	24027	40
Caelo	Benzoic acid	190752	24532	40

- 202 004 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 99 spectra from 71 *Apo-Ident* customers from 32 batches from the substance/substance group *Benzoic acid*.

- Among them are spectra of independent samples from 30 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
ACM	Benzoic acid	KNC0396J17	1
ACM	Benzoic acid	KNC0558J15	1
Anza	Benzoic acid	16001702	1
Anzag	Benzoic acid	16001708	1
Caelo	Benzoic acid	10156104	1
Caelo	Benzoic acid	13074605	3
Caelo	Benzoic acid	13074610	4
Caelo	Benzoic acid	1339120	1
Caelo	Benzoic acid	13391310	1
Caelo	Benzoic acid	13391314	1
Caelo	Benzoic acid	13391320	1
Caelo	Benzoic acid	15084603	3
Caelo	Benzoic acid	15084607	4
Caelo	Benzoic acid	15084614	2
Caelo	Benzoic acid	15084701	1
Caelo	Benzoic acid	16001702	2
Caelo	Benzoic acid	16001708	2
Caelo	Benzoic acid	16001714	7
Caelo	Benzoic acid	17327003	2
Caelo	Benzoic acid	17327004	1
Caelo	Benzoic acid	17327006	1
Caelo	Benzoic acid	17327009	2
Caelo	Benzoic acid	1732701	1
Caelo	Benzoic acid	17327013	6
Caelo	Benzoic acid	17327101	10
Caelo	Benzoic acid	190752005	1
Caelo	Benzoic acid	190752007	6
Caelo	Benzoic acid	20003734002	4
Caelo	Benzoic acid	20003734004	1
Caelo	Benzoic acid	20003734006	2
Caesar & Loretz GmbH...	Benzoic acid	17327013	2
Caesar & Loretz GmbH/Gehe	Benzoic acid	20003734004	1
Caesar & Loretz GmbH	Benzoic acid	17327003	2
Caesar & Loretz GmbH	Benzoic acid	17327006	2
Caesar & Loretz GmbH	Benzoic acid	17327009	1
Caesar & Loretz GmbH	Benzoic acid	17327013	1
Caesar & Loretz GmbH	Benzoic acid	190752007	1
Caesar & Loretz GmbH	Benzoic acid	20003734004	1
Caesar & Loretz GmbH	Benzoic acid	20003734006	1
Caesar & Loretz GmbH	Benzoic acid	20003734013	1
Caleo/Phoenix	Benzoic acid	15084607	1
Cealo, GEHE	Benzoic acid	20003734002	1
Cealo	Benzoic acid	13391314	1
Fresenius	Benzoic acid	80715102	1
Gatt-Koller / Phoenix	Benzoic acid	2992/07131314	2
Gehe	Benzoic acid	22001605009	1
Phönix	Benzoic acid	13074605	2
Phönix	Benzoic acid	16001714	1
Phönix	Benzoic acid	17327003	1
Sanacorp	Benzoic acid	16001714	1

- 235 968 spectra from 1515 *Apo-Ident* customers from a total of 49 226 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Benzoic acid* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Benzoic acid* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	80	0	202 004
Type C	0	99	0	235 968

The substance/substance group *Benzoic acid* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 93.9394 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21458	23096	17.95	116.71
22664	26693	16.00	116.50
23095	26693	14.86	116.10
23096	23096	0.00	119.78
23726	23096	8.30	119.51
26693	26693	0.00	120.91

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Benzydamine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20624-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Benzydamine hydrochloride; Benzydamini hydrochloridum

Special notes

When selecting the *Benzydamine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Benzydamine hydrochloride	6	7	89

Second-stage model

For differentiation of the substance/substance group *Benzydamine hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Benzydamine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Doxepin hydrochloride	59.69	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Benzydamine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Benzydamine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Benzydamine hydrochloride	AP300111801004B	24411	40	20180418
Euro OTC	Benzydamine hydrochloride	2011014	25596	40	20210310*
Euro OTC	Benzydamine hydrochloride	2011014-01	25781	50	20210317
Fagron	Benzydamine hydrochloride	14I30-B04-300713	21699	45	AR-15-FG-015977-01
Fagron	Benzydamine hydrochloride	15I17-B02-315060	22268	60	20151211
Fagron	Benzydamine hydrochloride	20K16-F04-375883	25718	50	20210105

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 285 spectra of 6 reference samples from the substance/substance group *Benzydamine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 677 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 370 spectra of 11 reference samples from the substance/substance group *Benzydamine hydrochloride*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Benzydamine hydrochloride	2201027	25967	40
Euro OTC	Benzydamine hydrochloride	2301015	26587	40
Euro OTC	Benzydamine hydrochloride	2401026	27372	40
Euro OTC	Benzydamine hydrochloride	2409005	27387	40
Fagron	Benzydamine hydrochloride	16D05-B50-332333	23203	40
Fagron	Benzydamine hydrochloride	17H01-B03-345050	23942	40
Fagron	Benzydamine hydrochloride	18H29-B02-355663	24445	40
Euro OTC	Benzydamine hydrochloride	2201027	25967SI	10
Euro OTC	Benzydamine hydrochloride	2301015	26587SI	20
Euro OTC	Benzydamine hydrochloride	2401026	27372SI	20
Fagron	Benzydamine hydrochloride	16D05-B50-332333	23204	40

- 201 714 spectra from a total of 4038 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 242 spectra from 195 *Apo-Ident* customers from 96 batches from the substance/substance group *Benzydamine hydrochloride*.

- Among them are spectra of independent samples from 88 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Benzydamine hydrochloride	2103302P	1
	Benzydamine hydrochloride	21G10-B09-213933	1
	Benzydamine hydrochloride	21G10-B10-213932	2
	Benzydamine hydrochloride	21G10B10219520	1
	Benzydamine hydrochloride	21G10-B10-219520	3
	Benzydamine hydrochloride	2201027-01	1
	Benzydamine hydrochloride	2201027-02	3
20E13-F02_373489	Benzydamine hydrochloride	Fagron	1
Anzag/ Audov	Benzydamine hydrochloride	AP300111801004B	1
Audor Pharma	Benzydamine hydrochloride	19K25-F01	1
Audor Pharma	Benzydamine hydrochloride	300111702007	1
Audor Pharma	Benzydamine hydrochloride	300111702007b	1
Audor Pharma	Benzydamine hydrochloride	300111702007B	1
Audor Pharma	Benzydamine hydrochloride	300111801004B	3
Audor Pharma	Benzydamine hydrochloride	AP3000111801004B	1
Audor Pharma	Benzydamine hydrochloride	AP300111702007	1
Audor Pharma	Benzydamine hydrochloride	AP300111702007B	6
Audor Pharma	Benzydamine hydrochloride	AP300111801004	1
Audor Pharma	Benzydamine hydrochloride	AP300111801004B	6
Bal Pharma	Benzydamine hydrochloride	AP300111801004B	1
Caelo	Benzydamine hydrochloride	12K07-N16	1
Caelo	Benzydamine hydrochloride	17H01-B03-345050	2
Caelo	Benzydamine hydrochloride	1803309P	1
Caelo	Benzydamine hydrochloride	18H29B02355663	1
Caelo	Benzydamine hydrochloride	18H29B02-358710	1
Caelo	Benzydamine hydrochloride	18H29-B02-358710	2
Caelo	Benzydamine hydrochloride	1903303P	1
Centaur / Gehe	Benzydamine hydrochloride	18H29-B02-361603	1
Euro OTC	Benzydamine hydrochloride	2001026-01	1
Euro OTC	Benzydamine hydrochloride	2011014-01	1
Fagron	Benzydamine hydrochloride		1
Fagron	Benzydamine hydrochloride	12C20-N02	1
Fagron	Benzydamine hydrochloride	12J10-N03	1
Fagron	Benzydamine hydrochloride	12K07-N16	1
Fagron	Benzydamine hydrochloride	13A15-N03	1
Fagron	Benzydamine hydrochloride	13H19_N06	1
Fagron	Benzydamine hydrochloride	13H19-N06	1
Fagron	Benzydamine hydrochloride	14B25-B01-294054	1
Fagron	Benzydamine hydrochloride	1503309P	1
Fagron	Benzydamine hydrochloride	1503313P	1
Fagron	Benzydamine hydrochloride	1503315P	1
Fagron	Benzydamine hydrochloride	15A14-B05	2
Fagron	Benzydamine hydrochloride	15A14-B05-303068	1
Fagron	Benzydamine hydrochloride	15A14-B05-307102	1
Fagron	Benzydamine hydrochloride	15A14-B05-307103	1
Fagron	Benzydamine hydrochloride	15I17-B02	1
Fagron	Benzydamine hydrochloride	16B09-B05-318272	3
Fagron	Benzydamine hydrochloride	16B09-B05-318273	2
Fagron	Benzydamine hydrochloride	16B09-B05-320007	1
Fagron	Benzydamine hydrochloride	16d05-b50-332333	1
Fagron	Benzydamine hydrochloride	16D05-B50-332333	1
Fagron	Benzydamine hydrochloride	16D05-b50-332334	1
Fagron	Benzydamine hydrochloride	16D05-B50-332334	3
Fagron	Benzydamine hydrochloride	1703305P	1
Fagron	Benzydamine hydrochloride	17H01-B03	1
Fagron	Benzydamine hydrochloride	17H01-B03_34641	1
Fagron	Benzydamine hydrochloride	17H01-B03-345050	5
Fagron	Benzydamine hydrochloride	17H01-B03-345051	2
Fagron	Benzydamine hydrochloride	17H01-B03-348469	4
Fagron	Benzydamine hydrochloride	17H01-B03-348470	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Benzydamine hydrochloride	1803309P	4
Fagron	Benzydamine hydrochloride	18H29-02-358710	1
Fagron	Benzydamine hydrochloride	18H29-B02	2
Fagron	Benzydamine hydrochloride	18H29-B02-354329	5
Fagron	Benzydamine hydrochloride	18H29-B02-354330	2
Fagron	Benzydamine hydrochloride	18H29-B02-355318	1
Fagron	Benzydamine hydrochloride	18H29-B02-355663	4
Fagron	Benzydamine hydrochloride	18H29-B02-357424	1
Fagron	Benzydamine hydrochloride	18H29-B02-358710	4
Fagron	Benzydamine hydrochloride	18H29-B02-358711	1
Fagron	Benzydamine hydrochloride	18H29-B02-361603	3
Fagron	Benzydamine hydrochloride	18H29-B-357424	1
Fagron	Benzydamine hydrochloride	1903303P	2
Fagron	Benzydamine hydrochloride	19K25-F01	3
Fagron	Benzydamine hydrochloride	19K25-F01_366695	1
Fagron	Benzydamine hydrochloride	19K25-F01-366695	10
Fagron	Benzydamine hydrochloride	19K25-F01-366697	2
Fagron	Benzydamine hydrochloride	19K25-F01-366699	6
Fagron	Benzydamine hydrochloride	19K25-FO1-366695	1
Fagron	Benzydamine hydrochloride	19K25-FO1-366699	1
Fagron	Benzydamine hydrochloride	2003305P	3
Fagron	Benzydamine hydrochloride	200330SP	1
Fagron	Benzydamine hydrochloride	2003311P	2
Fagron	Benzydamine hydrochloride	20E13-F02	9
Fagron	Benzydamine hydrochloride	20E13-F02-2373489	1
Fagron	Benzydamine hydrochloride	20E13-F02-373391	1
Fagron	Benzydamine hydrochloride	20E13-F02-373489	16
Fagron	Benzydamine hydrochloride	20E13-F02-373491	1
Fagron	Benzydamine hydrochloride	20K16-F04	1
Fagron	Benzydamine hydrochloride	2103302P	2
Fagron	Benzydamine hydrochloride	21G10-810-213932	2
Fagron	Benzydamine hydrochloride	21G10-B10	2
Fagron	Benzydamine hydrochloride	21G10-B10_213932	1
Fagron	Benzydamine hydrochloride	21G10-B10-2103932	1
Fagron	Benzydamine hydrochloride	21g10b10213932	1
Fagron	Benzydamine hydrochloride	21g10-b10-213932	1
Fagron	Benzydamine hydrochloride	21G10-B10-213932	22
Fagron	Benzydamine hydrochloride	21G10-B10-213932fagr	1
Fagron	Benzydamine hydrochloride	21G10-B10-219520	1
Fagron	Benzydamine hydrochloride	220830(21G10-B10-213932)	1
Fagron	Benzydamine hydrochloride	25021710	1
Fagron	Benzydamine hydrochloride	3280417	1
Fagron	Benzydamine hydrochloride	F02-3734809	5
Fargon/Noweda	Benzydamine hydrochloride	19K25-FO1-366695	1
Fargon	Benzydamine hydrochloride	21G10-B10-213932	1
Fragron	Benzydamine hydrochloride	18H29-B02-358711	1
Fresenius	Benzydamine hydrochloride	30062015099	1
Gehe	Benzydamine hydrochloride	18H29-B02-354329	1
Gehe	Benzydamine hydrochloride	21G10-B10-219520	1
Gehe	Benzydamine hydrochloride	AP300111801004B	1
GUMO	Benzydamine hydrochloride	19k25-f01	1
Noweda	Benzydamine hydrochloride	21G10-B10-219520	1
Phönix	Benzydamine hydrochloride	19K25-F01-366695	1
Phönix	Benzydamine hydrochloride	2003305P	1
Phönix	Benzydamine hydrochloride	f02-3734809	1
Sanacorp	Benzydamine hydrochloride	18H29-B02	1
SANACORP	Benzydamine hydrochloride	18H29-B02	1
Sanacorp	Benzydamine hydrochloride	18H29-Bo2-355663	1
Sanacorp	Benzydamine hydrochloride	20E13-F02-3734809	1
Sanacorp	Benzydamine hydrochloride	21G10-B10-213932	1

- 235 825 spectra from 1515 *Apo-Ident* customers from a total of 49 163 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Benzydamine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Benzydamine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	285	0	152 677
Type B	0	370	0	201 714
Type C	0	227	15	235 825

The substance/substance group *Benzydamine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8947 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.3784 %)
Type C	100.0000 % (> 99.9007 %)	93.8017 % (> 92.5620 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21699	21699	0.00	123.13
22268	21699	5.26	117.99
24411	25596	7.98	123.39
25596	25596	0.00	122.51
25718	21699	23.23	128.63
25781	25596	15.86	124.92

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Betaine monohydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20498-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Betaine monohydrate; Betainum monohydricum

Special notes

When selecting the *Betaine monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Betaine monohydrate	4	1	4

Second-stage model

For differentiation of the substance/substance group *Betaine monohydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Betaine monohydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	132.83	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Betaine monohydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Betaine monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Betaine monohydrate	12336602	20991	40	1403327
Fagron	Betaine monohydrate	14I26-B06-309878	21956	60	20141212
Fagron	Betaine monohydrate	18H13-B01-355585	24585	40	20180907
Fagron	Betaine monohydrate	20J26-B02-201459	25480	40	20201104

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 4 reference samples from the substance/substance group *Betaine monohydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 782 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Betaine monohydrate*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Betaine monohydrate	16H03-B04-330370	23092	40
Fagron	Betaine monohydrate	16H03-B04-330370	23378	40

- 202 004 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 3 *Apo-Ident* customers from 4 batches from the substance/substance group *Betaine monohydrate*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Betaine monohydrate	14A14-B02-292983	1
Caelo	Betaine monohydrate	4312172831	1
Fagron	Betaine monohydrate	16H03-B04	1
Fagron	Betaine monohydrate	16H03-B04-330370	1

- 236 063 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Betaine monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Betaine monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	180	0	152 782
Type B	0	80	0	202 004
Type C	0	4	0	236 063

The substance/substance group *Betaine monohydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20991	20991	0.00	271.72
21956	20991	6.48	271.34
24585	20991	11.29	266.66
25480	20991	13.89	271.81

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Betamethasone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20943-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Betamethasone; Betamethasonum

Special notes

When selecting the *Betamethasone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Betamethasone	5	3	38

Second-stage model

For differentiation of the substance/substance group *Betamethasone* the following second-stage model is used:

- Submodel 02

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Betamethasone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	91.24	–
⋮	⋮	⋮
Methylprednisolone	>50	52.42
Dexamethasone	>50	57.14
Fluocinolone acetonide	>50	58.62
Triamcinolone acetonide	>50	64.54
Prednisolone	>50	67.35
Tyrothricin	>50	90.23
Gramicidin	>50	153.50

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Betamethasone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Betamethasone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Betamethasone	12D26-N08	20943	40	1402096
Fagron	Betamethasone	13H08-N06	21579	60	1411037
Fagron	Betamethasone	11H31-B06-288219	22493	40	1608324
Fagron	Betamethasone	20A27-F07-368847	25173	40	20200320
Fagron	Betamethasone	23F15-B13-227908	26981	40	20230817

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 220 spectra of 5 reference samples from the substance/substance group *Betamethasone*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 742 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 4 reference samples from the substance/substance group *Betamethasone*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Betamethasone	14C13-B02-296165	22897	40
Fagron	Betamethasone	15L09-B05-324091	22904	40
Fagron	Betamethasone	21K15-B08-213853	26062	40
Fagron	Betamethasone	21K15-B08-213853	26062SI	40

- 201 924 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 53 spectra from 38 *Apo-Ident* customers from 40 batches from the substance/substance group *Betamethasone*.

- Among them are spectra of independent samples from 38 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
BASF/Phönix	Betamethasone	ZBtBY13004	1
Caelo	Betamethasone	11/14-N02	1
Caelo	Betamethasone	16l07-B01-341871	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Betamethasone	11/14-N02	1
Fagron	Betamethasone	11H31-B06-288217	1
Fagron	Betamethasone	12B20-N05	2
Fagron	Betamethasone	12D26-N08	1
Fagron	Betamethasone	12D26-NO8	1
Fagron	Betamethasone	12J01-N02	1
Fagron	Betamethasone	14C13-B02	2
Fagron	Betamethasone	14C13-B02-296154	1
Fagron	Betamethasone	14C13-B02-296164	2
Fagron	Betamethasone	14C13-B02-305561	1
Fagron	Betamethasone	14c13-bo2-305561	1
Fagron	Betamethasone	15L09-B05	1
Fagron	Betamethasone	15L09-B05_322119	1
Fagron	Betamethasone	16I07-B01-341871	3
Fagron	Betamethasone	1810B02-353535	1
Fagron	Betamethasone	18I10-B02-353535	1
Fagron	Betamethasone	18I10-B02-353536	2
Fagron	Betamethasone	18I10-B02-355063	2
Fagron	Betamethasone	18I10-B02-357418	1
Fagron	Betamethasone	18l10-B02-355063	1
Fagron	Betamethasone	20A27-F07	1
Fagron	Betamethasone	20A27-F07-368846	2
Fagron	Betamethasone	20A27-F07-368847	1
Fagron	Betamethasone	20A27-F07-370552	1
Fagron	Betamethasone	21K15-B08-213852	1
Fagron	Betamethasone	9071304	1
Fagron	Betamethasone	9J26-N08	1
Fagron	Betamethasone	9K25-N13	1
Fagron	Betamethasone	BT-191101	1
Fagron	Betamethasone	F07-3705501	1
Fagron	Betamethasone	ZBTBY15002	1
Fargon	Betamethasone	20A27-F07-370551	1
Fiebig	Betamethasone	12J01-120301-m1	1
Gehe amax	Betamethasone	18/10-B02-353535	1
Gehe	Betamethasone	15L09-B05-319353	1
Huan Yuxin Pharmaceutics	Betamethasone	20A27-F07-370551	1
Hunan Yuxin Pharmace…	Betamethasone	20A27-F07-372113	1
Noweda	Betamethasone	12B20-N05	1
Noweda	Betamethasone	M-XO1-120301m1	1
Phönix	Betamethasone	12B20-N05	1
Symbiotec Pharmalab …	Betamethasone	14C13-B02	1
Unisan	Betamethasone	Retest09K25-N13	1

- 236 014 spectra from 1515 *Apo-Ident* customers from a total of 49 218 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Betamethasone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Betamethasone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	220	0	152 742
Type B	0	160	0	201 924
Type C	0	48	5	236 014

The substance/substance group *Betamethasone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	90.5660 % (> 84.9057 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20943	20943	0.00	116.34
21579	21579	0.00	128.89
22493	22493	0.00	127.56
25173	21579	26.39	133.76
26981	21579	22.01	135.26

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Betamethasone dipropionate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20930-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Betamethasone dipropionate; Betamethasoni dipropionas

Special notes

When selecting the *Betamethasone dipropionate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Betamethasone dipropionate	7	14	284

Second-stage model

For differentiation of the substance/substance group *Betamethasone dipropionate* the following second-stage model is used:

- Submodel 15

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Betamethasone dipropionate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Beclometasone dipropionate	37.10	33.36
Clobetasol propionate	38.35	53.00

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Betamethasone dipropionate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Betamethasone dipropionate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Betamethasone dipropionate	13372501	21250	40	AR-15-FG-005428-01
Caelo	Betamethasone dipropionate	13236803	21366	50	20130730
Caelo	Betamethasone dipropionate	13236803	21367	40	20130730
Euro OTC	Betamethasone dipropionate	1311023-01	21716	60	1505455
Euro OTC	Betamethasone dipropionate	1601034	22372	45	20160204*
Euro OTC	Betamethasone dipropionate	2102001	25691	50	20210528*
Euro OTC	Betamethasone dipropionate	2102001	25691SI	50	20210528*
Fagron	Betamethasone dipropionate	13I17-N05	20930	40	1401377
Fagron	Betamethasone dipropionate	13I17-N05	20952	80	20130926
Fagron	Betamethasone dipropionate	16C04-B03-324513	22898	40	20160421
Fagron	Betamethasone dipropionate	16C04-B03-324513	22898SI	39	20160421

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 534 spectra of 11 reference samples from the substance/substance group *Betamethasone dipropionate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 428 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1293 spectra of 33 reference samples from the substance/substance group *Betamethasone dipropionate*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Betamethasone dipropionate	171059	23342	40
Caelo	Betamethasone dipropionate	173536	23839	40
Caelo	Betamethasone dipropionate	22001649001	26313	40
Euro OTC	Betamethasone dipropionate	1610014	22851	40
Euro OTC	Betamethasone dipropionate	1705020	23539	40
Euro OTC	Betamethasone dipropionate	1801045	24090	40
Euro OTC	Betamethasone dipropionate	1811007	24343	40
Euro OTC	Betamethasone dipropionate	1907034	24796	40
Euro OTC	Betamethasone dipropionate	2003057	25309	40
Euro OTC	Betamethasone dipropionate	2110005	25914	40
Euro OTC	Betamethasone dipropionate	2208030	26345	40
Euro OTC	Betamethasone dipropionate	2301013	26573	40
Euro OTC	Betamethasone dipropionate	2406016	27350	40
Fagron	Betamethasone dipropionate	21K24-B04-216140	26178	40
Caelo	Betamethasone dipropionate	13372501	21250SI†	45
Caelo	Betamethasone dipropionate	13236803	21366SI†	46
Caelo	Betamethasone dipropionate	13236803	21367SI†	60
Caelo	Betamethasone dipropionate	171059	23342SI	20
Caelo	Betamethasone dipropionate	173536	23839SI	25
Caelo	Betamethasone dipropionate	22001649001	26313SI	40
Euro OTC	Betamethasone dipropionate	1311023-01	21716SI†	46
Euro OTC	Betamethasone dipropionate	1601034	22372SI†	45

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Betamethasone dipropionate	1610014	22851SI	30
Euro OTC	Betamethasone dipropionate	1705020	23539SI	27
Euro OTC	Betamethasone dipropionate	1801045	24090SI	39
Euro OTC	Betamethasone dipropionate	1811007	24343SI	30
Euro OTC	Betamethasone dipropionate	1907034	24796SI	40
Euro OTC	Betamethasone dipropionate	2003057	25309SI	40
Euro OTC	Betamethasone dipropionate	2110005	25914SI	40
Euro OTC	Betamethasone dipropionate	2208030	26345SI	40
Euro OTC	Betamethasone dipropionate	2301013	26573SI	40
Euro OTC	Betamethasone dipropionate	2406016	27350SI	40
Fagron	Betamethasone dipropionate	21K24-B04-216140	26178SI	40

- 200 791 spectra from a total of 4027 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1624 spectra from 648 *Apo-Ident* customers from 302 batches from the substance/substance group *Betamethasone dipropionate*.

- Among them are spectra of independent samples from 284 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Betamethasone dipropionate		1
	Betamethasone dipropionate	13/17-N05	2
	Betamethasone dipropionate	2110005-01	1
	Betamethasone dipropionate	21H18-B04-213656	1
	Betamethasone dipropionate	21K24-B04-220120	1
	Betamethasone dipropionate	21K24-B04-227289	1
	Betamethasone dipropionate	21K24-B04-227290	1
	Betamethasone dipropionate	22001649003	1
	Betamethasone dipropionate	22001649007	4
	Betamethasone dipropionate	22001649008	5
	Betamethasone dipropionate	22001649009	2
	Betamethasone dipropionate	22003962001	2
	Betamethasone dipropionate	22003962002	8
	Betamethasone dipropionate	2208030-01	7
	Betamethasone dipropionate	228030-01	1
	Betamethasone dipropionate	2301013-01	2
AHD/Caesar & Loretz GmbH	Betamethasone dipropionate	21000648013	1
AHD	Betamethasone dipropionate	18B06-B05-346219	1
Alliance Health 24.0...	Betamethasone dipropionate	13/17-N05	1
Alliance	Betamethasone dipropionate	22003962001	2
Anzag	Betamethasone dipropionate	12114513	2
Bombastus	Betamethasone dipropionate	12B27N08	1
cae	Betamethasone dipropionate	17353601	1
Cae	Betamethasone dipropionate	18293408	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Betamethasone dipropionate		2
Caelo	Betamethasone dipropionate	1210020-01	1
Caelo	Betamethasone dipropionate	12114501	1
Caelo	Betamethasone dipropionate	12114506	1
Caelo	Betamethasone dipropionate	12114507	2
Caelo	Betamethasone dipropionate	12114511	2
Caelo	Betamethasone dipropionate	12114512	1
Caelo	Betamethasone dipropionate	12114513	1
Caelo	Betamethasone dipropionate	13/17-N05	2
Caelo	Betamethasone dipropionate	13023001	3
Caelo	Betamethasone dipropionate	13023002	5
Caelo	Betamethasone dipropionate	13023002NP	1
Caelo	Betamethasone dipropionate	13023005	7
Caelo	Betamethasone dipropionate	1303006-01	1
Caelo	Betamethasone dipropionate	13125701	3
Caelo	Betamethasone dipropionate	13125703	5
Caelo	Betamethasone dipropionate	13236801	6
Caelo	Betamethasone dipropionate	13236801ok	1
Caelo	Betamethasone dipropionate	13236802	4
Caelo	Betamethasone dipropionate	13236803	1
Caelo	Betamethasone dipropionate	13236805	5
Caelo	Betamethasone dipropionate	13236806	3
Caelo	Betamethasone dipropionate	1325702	1
Caelo	Betamethasone dipropionate	13372501	3
Caelo	Betamethasone dipropionate	13372503	7
Caelo	Betamethasone dipropionate	13372504	5
Caelo	Betamethasone dipropionate	13372512	1
Caelo	Betamethasone dipropionate	13372514	12
Caelo	Betamethasone dipropionate	13372515	3
Caelo	Betamethasone dipropionate	13372516	4
Caelo	Betamethasone dipropionate	13372520	2
Caelo	Betamethasone dipropionate	140507	1
Caelo	Betamethasone dipropionate	14C03-B06-296837	1
Caelo	Betamethasone dipropionate	1503003-01	2
Caelo	Betamethasone dipropionate	1503003-02	1
Caelo	Betamethasone dipropionate	150605BD	1
Caelo	Betamethasone dipropionate	15163204	1
Caelo	Betamethasone dipropionate	15163301	15
Caelo	Betamethasone dipropionate	15163302	6
Caelo	Betamethasone dipropionate	15163303	12
Caelo	Betamethasone dipropionate	15163304	14
Caelo	Betamethasone dipropionate	15163305	1
Caelo	Betamethasone dipropionate	15238701	32
Caelo	Betamethasone dipropionate	15412901	1
Caelo	Betamethasone dipropionate	15412903	2
Caelo	Betamethasone dipropionate	15412905	1
Caelo	Betamethasone dipropionate	15412906	12
Caelo	Betamethasone dipropionate	15412907	5
Caelo	Betamethasone dipropionate	15412909	1
Caelo	Betamethasone dipropionate	15412910	7
Caelo	Betamethasone dipropionate	15412913	1
Caelo	Betamethasone dipropionate	15412914	7
Caelo	Betamethasone dipropionate	15412915	2
Caelo	Betamethasone dipropionate	15412916	1
Caelo	Betamethasone dipropionate	15H28-B06	1
Caelo	Betamethasone dipropionate	15H28B06313088	1
Caelo	Betamethasone dipropionate	15H28-B06-313088	1
Caelo	Betamethasone dipropionate	15-H28-B06-313088	1
Caelo	Betamethasone dipropionate	17015905	1
Caelo	Betamethasone dipropionate	1705020-01	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Betamethasone dipropionate	17105901	19
Caelo	Betamethasone dipropionate	17105902	17
Caelo	Betamethasone dipropionate	17105903	1
Caelo	Betamethasone dipropionate	17105905	4
Caelo	Betamethasone dipropionate	17105906	16
Caelo	Betamethasone dipropionate	17105907	10
Caelo	Betamethasone dipropionate	17105909	3
Caelo	Betamethasone dipropionate	17105911	6
Caelo	Betamethasone dipropionate	17353601	20
Caelo	Betamethasone dipropionate	17353603	16
Caelo	Betamethasone dipropionate	1735601	1
Caelo	Betamethasone dipropionate	17B16-B04	1
Caelo	Betamethasone dipropionate	17B16-B04-332220	1
Caelo	Betamethasone dipropionate	17E22-B06-336993	1
Caelo	Betamethasone dipropionate	17H16B04340537	1
Caelo	Betamethasone dipropionate	1801045-01	3
Caelo	Betamethasone dipropionate	18041819	1
Caelo	Betamethasone dipropionate	18090601	7
Caelo	Betamethasone dipropionate	18090602	7
Caelo	Betamethasone dipropionate	18090603	13
Caelo	Betamethasone dipropionate	18090606	22
Caelo	Betamethasone dipropionate	18090607	14
Caelo	Betamethasone dipropionate	18090608	15
Caelo	Betamethasone dipropionate	1811007-01	2
Caelo	Betamethasone dipropionate	18121306	1
Caelo	Betamethasone dipropionate	18292406	1
Caelo	Betamethasone dipropionate	18293402	12
Caelo	Betamethasone dipropionate	18293404	14
Caelo	Betamethasone dipropionate	182934046	1
Caelo	Betamethasone dipropionate	18293406	26
Caelo	Betamethasone dipropionate	18293407	4
Caelo	Betamethasone dipropionate	18293408	26
Caelo	Betamethasone dipropionate	18294306	1
Caelo	Betamethasone dipropionate	18B06-B05-350473	2
Caelo	Betamethasone dipropionate	18B06-B05-352731	1
Caelo	Betamethasone dipropionate	19000537003	10
Caelo	Betamethasone dipropionate	19000537007	24
Caelo	Betamethasone dipropionate	19000537008	5
Caelo	Betamethasone dipropionate	19000537010	10
Caelo	Betamethasone dipropionate	1900537008	1
Caelo	Betamethasone dipropionate	1900537010	1
Caelo	Betamethasone dipropionate	1907034-01	1
Caelo	Betamethasone dipropionate	20003997001	7
Caelo	Betamethasone dipropionate	20003997002	8
Caelo	Betamethasone dipropionate	20003997005	14
Caelo	Betamethasone dipropionate	2000648010	1
Caelo	Betamethasone dipropionate	21000645001	2
Caelo	Betamethasone dipropionate	21000648001	1
Caelo	Betamethasone dipropionate	21000648002	4
Caelo	Betamethasone dipropionate	21000648003	5
Caelo	Betamethasone dipropionate	21000648004	5
Caelo	Betamethasone dipropionate	21000648006	3
Caelo	Betamethasone dipropionate	21000648007	11
Caelo	Betamethasone dipropionate	21000648010	10
Caelo	Betamethasone dipropionate	21000648012	2
Caelo	Betamethasone dipropionate	21000648013	8
Caelo	Betamethasone dipropionate	21000648014	4
Caelo	Betamethasone dipropionate	2100648006	1
Caelo	Betamethasone dipropionate	2109DMOB00111322	1
Caelo	Betamethasone dipropionate	21648004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Betamethasone dipropionate	22001649001	13
Caelo	Betamethasone dipropionate	22001649002	10
Caelo	Betamethasone dipropionate	22001649003	1
Caelo	Betamethasone dipropionate	22001649005	3
Caelo	Betamethasone dipropionate	22001649007	2
Caelo	Betamethasone dipropionate	22001649008	1
Caelo	Betamethasone dipropionate	22003962002	1
Caelo	Betamethasone dipropionate	220621(21000648014)	1
Caelo	Betamethasone dipropionate	3170717	1
Caelo	Betamethasone dipropionate	700216-0001	1
Caelo	Betamethasone dipropionate	8K03-N13	1
Caelo	Betamethasone dipropionate	AKD11	1
Caesar & Loretz GmbH...	Betamethasone dipropionate	18293406	1
Caesar & Loretz GmbH...	Betamethasone dipropionate	18293402	1
Caesar & Loretz GmbH...	Betamethasone dipropionate	18293408	1
Caesar & Loretz GmbH...	Betamethasone dipropionate	18090603	1
Caesar & Loretz GmbH...	Betamethasone dipropionate	22001649005	1
Caesar & Loretz GmbH...	Betamethasone dipropionate	18293408	1
Caesar & Loretz GmbH...	Betamethasone dipropionate	22001649005	1
Caesar & Loretz GmbH...	Betamethasone dipropionate	21000648013	1
Caesar & Loretz GmbH...	Betamethasone dipropionate	21000648007	1
Caesar & Loretz GmbH...	Betamethasone dipropionate	19000537003	1
Caesar & Loretz GmbH...	Betamethasone dipropionate	18293408	1
Caesar & Loretz GmbH/Gehe	Betamethasone dipropionate	18090606	2
Caesar & Loretz GmbH/Gehe	Betamethasone dipropionate	19000537003	1
Caesar & Loretz GmbH/Gehe	Betamethasone dipropionate	20003997001	1
Caesar & Loretz GmbH/Gehe	Betamethasone dipropionate	21000648006	2
Caesar & Loretz GmbH/Gehe	Betamethasone dipropionate	21000648010	1
Caesar & Loretz GmbH/K	Betamethasone dipropionate	21000648013	1
Caesar & Loretz GmbH...	Betamethasone dipropionate	18090602	2
Caesar & Loretz GmbH...	Betamethasone dipropionate	19000537010	2
Caesar & Loretz GmbH...	Betamethasone dipropionate	20003997005	2
Caesar & Loretz GmbH...	Betamethasone dipropionate	20003997002	1
Caesar & Loretz GmbH...	Betamethasone dipropionate	21000648004	1
Caesar & Loretz GmbH/S	Betamethasone dipropionate	21000648007	1
Caesar & Loretz GmbH/S	Betamethasone dipropionate	22001649002	1
Caesar & Loretz GmbH...	Betamethasone dipropionate	18293406	3
Caesar & Loretz GmbH...	Betamethasone dipropionate	21000648007	1
Caesar & Loretz GmbH...	Betamethasone dipropionate	21000648014	1
Caesar & Loretz GmbH	Betamethasone dipropionate	17105902	1
Caesar & Loretz GmbH	Betamethasone dipropionate	17353605	1
Caesar & Loretz GmbH	Betamethasone dipropionate	18090606	2
Caesar & Loretz GmbH	Betamethasone dipropionate	18090608	1
Caesar & Loretz GmbH	Betamethasone dipropionate	18293402	3
Caesar & Loretz GmbH	Betamethasone dipropionate	18293404	5
Caesar & Loretz GmbH	Betamethasone dipropionate	18293406	8
Caesar & Loretz GmbH	Betamethasone dipropionate	18293407	1
Caesar & Loretz GmbH	Betamethasone dipropionate	18293408	7
Caesar & Loretz GmbH	Betamethasone dipropionate	19000537003	4
Caesar & Loretz GmbH	Betamethasone dipropionate	19000537007	6
Caesar & Loretz GmbH	Betamethasone dipropionate	19000537008	2
Caesar & Loretz GmbH	Betamethasone dipropionate	19000537010	1
Caesar & Loretz GmbH	Betamethasone dipropionate	20003997001	5
Caesar & Loretz GmbH	Betamethasone dipropionate	20003997002	3
Caesar & Loretz GmbH	Betamethasone dipropionate	20003997005	11
Caesar & Loretz GmbH	Betamethasone dipropionate	21000648001	2
Caesar & Loretz GmbH	Betamethasone dipropionate	21000648002	7
Caesar & Loretz GmbH	Betamethasone dipropionate	21000648003	3
Caesar & Loretz GmbH	Betamethasone dipropionate	21000648004	4
Caesar & Loretz GmbH	Betamethasone dipropionate	21000648006	8

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Betamethasone dipropionate	21000648007	2
Caesar & Loretz GmbH	Betamethasone dipropionate	21000648010	3
Caesar & Loretz GmbH	Betamethasone dipropionate	21000648012	3
Caesar & Loretz GmbH	Betamethasone dipropionate	21000648013	2
Caesar & Loretz GmbH	Betamethasone dipropionate	21000648014	2
Caesar & Loretz GmbH	Betamethasone dipropionate	22001649001	6
Caesar & Loretz GmbH	Betamethasone dipropionate	22001649002	3
Caesar & Loretz Hild...	Betamethasone dipropionate	18293408	1
Caesar & Loretz Hilden	Betamethasone dipropionate	18293404	1
Caesar & Loretz Hilden	Betamethasone dipropionate	18293406	1
Caesar & Loretz Hilden	Betamethasone dipropionate	19000537007	1
Caesar & Loretz	Betamethasone dipropionate	22001649002	1
Caesar & Loretz	Betamethasone dipropionate	22001649005	1
Cealo / Otto Geilenk...	Betamethasone dipropionate	18293402	1
Cealo/ AHD	Betamethasone dipropionate	18293402	1
Cealo/Sanacorp	Betamethasone dipropionate	13125701	1
Cealo	Betamethasone dipropionate	17353601	1
Crystal Pharma / Ebert	Betamethasone dipropionate	15163301	1
Crystal Pharma / Gehe	Betamethasone dipropionate	17105906	1
Delta	Betamethasone dipropionate	18B06-B05-346219	1
EU RHO/GEHE	Betamethasone dipropionate	2003057-01	1
EuRho/ Noweda	Betamethasone dipropionate	2003057-01	1
EuRho/ Noweda	Betamethasone dipropionate	2208030-01	1
EuRho/Alliance	Betamethasone dipropionate	2003057-01	1
EuRho/Fiebig	Betamethasone dipropionate	1811007-01	1
EuRho/Noweda	Betamethasone dipropionate	1907034-01	2
EuRho/Phoenix	Betamethasone dipropionate	2102001-01	1
Eurho/Phönix	Betamethasone dipropionate		1
EuRho/Phönix	Betamethasone dipropionate	2003057-01	1
euro AHD	Betamethasone dipropionate	1801045-015715	1
euro AHD	Betamethasone dipropionate	1801045-015787	1
Euro OTC	Betamethasone dipropionate	102001-012	1
Euro OTC	Betamethasone dipropionate	111007-01	1
Euro OTC	Betamethasone dipropionate	121002001	1
Euro OTC	Betamethasone dipropionate	1303006/01	1
Euro OTC	Betamethasone dipropionate	1303006-01	2
Euro OTC	Betamethasone dipropionate	1303006-02	1
Euro OTC	Betamethasone dipropionate	1305041-01	10
Euro OTC	Betamethasone dipropionate	1305041-02	3
Euro OTC	Betamethasone dipropionate	130541-01	1
Euro OTC	Betamethasone dipropionate	131023-02	1
Euro OTC	Betamethasone dipropionate	131102301	2
Euro OTC	Betamethasone dipropionate	1311023-01	11
Euro OTC	Betamethasone dipropionate	1311023-02	5
Euro OTC	Betamethasone dipropionate	13125702	1
Euro OTC	Betamethasone dipropionate	13372501	1
Euro OTC	Betamethasone dipropionate	1503003-01	10
Euro OTC	Betamethasone dipropionate	150300302	1
Euro OTC	Betamethasone dipropionate	1503003-02	12
Euro OTC	Betamethasone dipropionate	1506016-02	1
Euro OTC	Betamethasone dipropionate	15163304	1
Euro OTC	Betamethasone dipropionate	153003-01	1
Euro OTC	Betamethasone dipropionate	160103401	1
Euro OTC	Betamethasone dipropionate	1601034-01	25
Euro OTC	Betamethasone dipropionate	1610014-01	37
Euro OTC	Betamethasone dipropionate	1610014-015308	1
Euro OTC	Betamethasone dipropionate	17050-01	1
Euro OTC	Betamethasone dipropionate	170502001	1
Euro OTC	Betamethasone dipropionate	1705020-01	25
Euro OTC	Betamethasone dipropionate	17B16-B04-332218	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Betamethasone dipropionate	180104501	3
Euro OTC	Betamethasone dipropionate	1801045-01	27
Euro OTC	Betamethasone dipropionate	180808185	1
Euro OTC	Betamethasone dipropionate	1811007	1
Euro OTC	Betamethasone dipropionate	181100701	2
Euro OTC	Betamethasone dipropionate	1811007-01	25
Euro OTC	Betamethasone dipropionate	19070324-01	1
Euro OTC	Betamethasone dipropionate	1907034	1
Euro OTC	Betamethasone dipropionate	190703401	1
Euro OTC	Betamethasone dipropionate	1907034-01	32
Euro OTC	Betamethasone dipropionate	1907234-01	1
Euro OTC	Betamethasone dipropionate	20030057-01	1
Euro OTC	Betamethasone dipropionate	2003024-01	1
Euro OTC	Betamethasone dipropionate	200305-01	1
Euro OTC	Betamethasone dipropionate	2003057	1
Euro OTC	Betamethasone dipropionate	2003057-01	31
Euro OTC	Betamethasone dipropionate	2102001-01	21
Euro OTC	Betamethasone dipropionate	211000-01	1
Euro OTC	Betamethasone dipropionate	2110005-01	15
Euro OTC	Betamethasone dipropionate	2110005-02	5
Euro OTC	Betamethasone dipropionate	2208030-01	12
Euro OTC	Betamethasone dipropionate	2208030-1	1
Euro OTC	Betamethasone dipropionate	2208630-01	1
Euro OTC	Betamethasone dipropionate	BDP102/0817	1
Euro OTC	Betamethasone dipropionate	C0044/1A170130	1
euro//Noweda	Betamethasone dipropionate	1705030-01	1
EUro/AHD	Betamethasone dipropionate	1303006-01	3
Euro/Gehe	Betamethasone dipropionate	1601034-01	1
Euro/Gehe	Betamethasone dipropionate	2102001	1
Euro/Krieger	Betamethasone dipropionate	1801045-01	1
Euro/Phönix	Betamethasone dipropionate	2208030-01	1
Euro/Sanacorp	Betamethasone dipropionate	1503003-02	1
Fagon/Noweda	Betamethasone dipropionate	18I27-B03	1
Fagron	Betamethasone dipropionate		7
Fagron	Betamethasone dipropionate	10E19-N03	1
Fagron	Betamethasone dipropionate	11D26-N06	2
Fagron	Betamethasone dipropionate	11I02-N01	1
Fagron	Betamethasone dipropionate	11K28-N10	2
Fagron	Betamethasone dipropionate	12827-N08	1
Fagron	Betamethasone dipropionate	12B27-N08	6
Fagron	Betamethasone dipropionate	12C21-N13	1
Fagron	Betamethasone dipropionate	13/17-n05	1
Fagron	Betamethasone dipropionate	13/17-N05	15
Fagron	Betamethasone dipropionate	13023004	1
Fagron	Betamethasone dipropionate	1317-N05	1
Fagron	Betamethasone dipropionate	13i17-N05	1
Fagron	Betamethasone dipropionate	13I17-N05	12
Fagron	Betamethasone dipropionate	13j16-B01-291844	1
Fagron	Betamethasone dipropionate	13j16-b01-291845	1
Fagron	Betamethasone dipropionate	13J16-B01-291845	2
Fagron	Betamethasone dipropionate	14C03-B03-296838	1
Fagron	Betamethasone dipropionate	14C03-B06	2
Fagron	Betamethasone dipropionate	14C03-B06-296837	10
Fagron	Betamethasone dipropionate	15H25-B06-313088	1
Fagron	Betamethasone dipropionate	15H28B06313088	1
Fagron	Betamethasone dipropionate	15H28-B06-313088	4
Fagron	Betamethasone dipropionate	1601034-01	1
Fagron	Betamethasone dipropionate	16C04-B03	1
Fagron	Betamethasone dipropionate	16C04-B03-320850	5
Fagron	Betamethasone dipropionate	16C04-B03-320851	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Betamethasone dipropionate	16C04-B03-320852	1
Fagron	Betamethasone dipropionate	17816B04332224	1
Fagron	Betamethasone dipropionate	17B16-B04	1
Fagron	Betamethasone dipropionate	17B16-B04-332217	9
Fagron	Betamethasone dipropionate	17b16b04332218	1
Fagron	Betamethasone dipropionate	17B16-B04-332219-201	1
Fagron	Betamethasone dipropionate	17B16-B04-332224	4
Fagron	Betamethasone dipropionate	17B6-B04-332217	1
Fagron	Betamethasone dipropionate	17E22-B06-335244	3
Fagron	Betamethasone dipropionate	17E22-B06-336705	2
Fagron	Betamethasone dipropionate	17E22B06336993	1
Fagron	Betamethasone dipropionate	17E22-B06-336993	5
Fagron	Betamethasone dipropionate	17H16-B04-340537	1
Fagron	Betamethasone dipropionate	18/27-B03-357221	2
Fagron	Betamethasone dipropionate	1801045-01	1
Fagron	Betamethasone dipropionate	1811007-01	1
Fagron	Betamethasone dipropionate	18127-B03-362601	1
Fagron	Betamethasone dipropionate	18127-B03-362603	1
Fagron	Betamethasone dipropionate	1827-b03-362601	1
Fagron	Betamethasone dipropionate	18B06-B05	5
Fagron	Betamethasone dipropionate	18B06-B05_350473	1
Fagron	Betamethasone dipropionate	18B06-B05-346218	5
Fagron	Betamethasone dipropionate	18B06-B05-346219	1
Fagron	Betamethasone dipropionate	18B06B05347338	1
Fagron	Betamethasone dipropionate	18B06-B05-347338	5
Fagron	Betamethasone dipropionate	18B06B0534996	1
Fagron	Betamethasone dipropionate	18b06-b05-350473	1
Fagron	Betamethasone dipropionate	18B06-B05-350473	10
Fagron	Betamethasone dipropionate	18B06-B05-350474	1
Fagron	Betamethasone dipropionate	18B06B05352731	2
Fagron	Betamethasone dipropionate	18B06-B05-352731	5
Fagron	Betamethasone dipropionate	18B06B05354807	1
Fagron	Betamethasone dipropionate	18B06-B05-354807	6
Fagron	Betamethasone dipropionate	18B06-B05-354808	3
Fagron	Betamethasone dipropionate	18Bo6-B0o5-352731	1
Fagron	Betamethasone dipropionate	18I127-B03-357222	1
Fagron	Betamethasone dipropionate	18I27-B03	8
Fagron	Betamethasone dipropionate	18I27-B03-357221	4
Fagron	Betamethasone dipropionate	18I27-B03-357222	3
Fagron	Betamethasone dipropionate	18I27-B03-358725	3
Fagron	Betamethasone dipropionate	18I27-B03-358726	1
Fagron	Betamethasone dipropionate	18I27-B03-358727	1
Fagron	Betamethasone dipropionate	18I27-B03-3626001	1
Fagron	Betamethasone dipropionate	18I27-B03-362601	10
Fagron	Betamethasone dipropionate	18I27-B03-362602	2
Fagron	Betamethasone dipropionate	18I27-BO3-362602	1
Fagron	Betamethasone dipropionate	18l27-B03-358725	1
Fagron	Betamethasone dipropionate	19041706	1
Fagron	Betamethasone dipropionate	19J31-F02	3
Fagron	Betamethasone dipropionate	19J31-F02-3666808	1
Fagron	Betamethasone dipropionate	19J31F02-366807	1
Fagron	Betamethasone dipropionate	19J31-F02-366807	7
Fagron	Betamethasone dipropionate	19J31-F02-366808	9
Fagron	Betamethasone dipropionate	19J31-F02-366809	1
Fagron	Betamethasone dipropionate	19J31-F02-366810	2
Fagron	Betamethasone dipropionate	20171127Ma5	1
Fagron	Betamethasone dipropionate	20C10_F02372115	1
Fagron	Betamethasone dipropionate	20C10-F02	1
Fagron	Betamethasone dipropionate	20C10-F02372115	1
Fagron	Betamethasone dipropionate	20C10-F02-372115	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Betamethasone dipropionate	2109DM0B0011322	1
Fagron	Betamethasone dipropionate	21C002-F01-377438	1
Fagron	Betamethasone dipropionate	21C02-F01-3774308	1
Fagron	Betamethasone dipropionate	21C02-F01-377438	1
Fagron	Betamethasone dipropionate	21H18-B04-213656	8
Fagron	Betamethasone dipropionate	21J12-B09-216139	6
Fagron	Betamethasone dipropionate	21K24B04216140	2
Fagron	Betamethasone dipropionate	21K24-B04-216140	1
Fagron	Betamethasone dipropionate	21K24-B04-220120	2
Fagron	Betamethasone dipropionate	21K24-B04-222402	1
Fagron	Betamethasone dipropionate	21K24-B04-227289	2
Fagron	Betamethasone dipropionate	8K03-N13	1
Fagron	Betamethasone dipropionate	9J05-N09	1
Fagron	Betamethasone dipropionate	B03-3587205	1
Fagron	Betamethasone dipropionate	BDP003/0521	2
Fagron	Betamethasone dipropionate	BDP004/0821	1
Fagron	Betamethasone dipropionate	BDP101/0417	1
Fagron	Betamethasone dipropionate	BDP101/0419	2
Fagron	Betamethasone dipropionate	BDP102/0817	3
Fagron	Betamethasone dipropionate	F01-3774308	1
Fagron	Betamethasone dipropionate	F02-0668007	1
Fagron	Betamethasone dipropionate	F02-3668007	1
Fagron	Betamethasone dipropionate	F02-3721105	1
Fargon/ Noweda	Betamethasone dipropionate	13/17-N05	1
Fargon/AllianceH.	Betamethasone dipropionate	17H16B04-340537	1
Fargon	Betamethasone dipropionate	16C04-B033-24513	1
Fargon	Betamethasone dipropionate	17b16-b04-332224	1
Fragon/ Gehe	Betamethasone dipropionate	18B06-B05	1
Fragon	Betamethasone dipropionate	18B06-B05-352731	1
Gehe amax	Betamethasone dipropionate	1610014-01	1
Gehe amax	Betamethasone dipropionate	17B16-B04-332217	1
Gehe	Betamethasone dipropionate	1311023-01	1
Gehe	Betamethasone dipropionate	15238701	1
GEHE	Betamethasone dipropionate	15412914	1
Gehe	Betamethasone dipropionate	1705020-01	1
Gehe	Betamethasone dipropionate	17E22B06-336993	1
Gehe	Betamethasone dipropionate	18293404	1
GEHE	Betamethasone dipropionate	20003997005	1
Gehe	Betamethasone dipropionate	21000648001	1
Gehe	Betamethasone dipropionate	21000648010	1
Gehe	Betamethasone dipropionate	21000648012	1
Gehe	Betamethasone dipropionate	21k24-B04	1
Hirsch	Betamethasone dipropionate	1303006-01	1
Kehr	Betamethasone dipropionate	1705020-01	1
Kehr	Betamethasone dipropionate	220039602001	1
Klosterring	Betamethasone dipropionate	17B16-B04-332219	2
Nachprüfung	Betamethasone dipropionate	17B16-B04-332217	1
Noweda/ Caesar&Loren...	Betamethasone dipropionate	19000537003	1
Noweda	Betamethasone dipropionate	13236802	1
Noweda	Betamethasone dipropionate	13236803	1
Noweda	Betamethasone dipropionate	1811007-01	1
Noweda	Betamethasone dipropionate	21C02-F01-377438	1
Noweda	Betamethasone dipropionate	22001649008	1
Noweda	Betamethasone dipropionate	23011013-01	1
Noweda	Betamethasone dipropionate	BDP014/1115	1
Noweda	Betamethasone dipropionate	BDP102/0817	1
Ph/Euro	Betamethasone dipropionate	2110005-01	1
Phoenix 03.04.20147	Betamethasone dipropionate	13236805	1
Phoenix	Betamethasone dipropionate	13236806	1
Phoenix	Betamethasone dipropionate	1610014-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Betamethasone dipropionate	1705020-01	1
Phoenix	Betamethasone dipropionate	1811007-01	1
Phoenix	Betamethasone dipropionate	21000648006	1
Phönix Gotha	Betamethasone dipropionate	1811007-01	1
phönix	Betamethasone dipropionate	15163304	1
Phönix	Betamethasone dipropionate	1705020-01	1
PHÖNIX	Betamethasone dipropionate	17353603	1
Phönix	Betamethasone dipropionate	2003057-01	1
phönix	Betamethasone dipropionate	21000648014	1
Phönix	Betamethasone dipropionate	22001649005	1
sanacorb	Betamethasone dipropionate	12B27-No8	1
Sanacorp WE: 12.08.1...	Betamethasone dipropionate	15238701	1
Sanacorp	Betamethasone dipropionate	15412910	1
Sanacorp	Betamethasone dipropionate	1610014-01	1
Sanacorp	Betamethasone dipropionate	170502001	1
Sanacorp	Betamethasone dipropionate	1705020-01	1
Sanacorp	Betamethasone dipropionate	17105911	1
Sanacorp	Betamethasone dipropionate	17B16-B04-332217	2
Sanacorp	Betamethasone dipropionate	18090607	1
SANACORP	Betamethasone dipropionate	18293404	1
Sanacorp	Betamethasone dipropionate	18B06-B05-346218	1
Sanacorp	Betamethasone dipropionate	19000537010	1
Sanacorp	Betamethasone dipropionate	21000648010	1
Sanacorp	Betamethasone dipropionate	BDP102/0817	1
Symbiotica/Noweda	Betamethasone dipropionate	BDP102/0817	1
Symbiotica	Betamethasone dipropionate	2003057-01	2
Symbiotica	Betamethasone dipropionate	2208030-01	1
Symbiotica	Betamethasone dipropionate	BDP103/1019	1
WE:05.04.2016 Phönix	Betamethasone dipropionate	15163304	4
WE:09.12.2016	Betamethasone dipropionate	15163301	1

- 234 443 spectra from 1515 *Apo-Ident* customers from a total of 48 962 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Betamethasone dipropionate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Betamethasone dipropionate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	534	0	152 428
Type B	0	1293	0	200 791
Type C	0	1551	73	234 443

The substance/substance group *Betamethasone dipropionate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8764 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.5360 %)
Type C	100.0000 % (> 99.9007 %)	95.5049 % (> 95.3202 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20930	20930	0.00	39.63
20952	22372	8.46	38.31
21250	21250	0.00	38.12
21366	21250	5.41	38.46
21367	21250	5.99	39.15
21716	21716	0.00	38.96
22372	22372	0.00	37.10
22898	22372	7.89	39.40
25691	25691	0.00	42.14

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Betamethasone valerate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20026-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Betamethasone valerate; Betamethasoni valeras

Special notes

When selecting the *Betamethasone valerate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Betamethasone valerate	10	12	809

Second-stage model

For differentiation of the substance/substance group *Betamethasone valerate* the following second-stage model is used:

- Submodel 07

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Betamethasone valerate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prednisolon dihydrogen phosphate di…	80.71	–
⋮	⋮	⋮
Budesonide	>50	34.77
Erythromycin	>50	35.66

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Betamethasone valerate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Betamethasone valerate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Betamethasone valerate	13091213	21215	40	20130506
Caelo	Betamethasone valerate	13225507	21588	54	1706018
Euro OTC	Betamethasone valerate	1208014-01	20920	40	20120928
Euro OTC	Betamethasone valerate	1406019-01	21645	60	20140725
Euro OTC	Betamethasone valerate	1510037	22249	60	20151215*
Euro OTC	Betamethasone valerate	1510037	22249SI	30	20151215*
Euro OTC	Betamethasone valerate	1610010	22861	40	20161116*
Euro OTC	Betamethasone valerate	1811008	24349	40	20181207*
Euro OTC	Betamethasone valerate	1811008	24349SI	30	20181207*
Fagron	Betamethasone valerate	12K07-N23	20887	40	20121119
Fagron	Betamethasone valerate	13K29-B32-288243	21566	60	20131210
Fagron	Betamethasone valerate	13K05-B08-292651	21674	60	1511154

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 554 spectra of 12 reference samples from the substance/substance group *Betamethasone valerate*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 408 spectra from a total of 2832 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 881 spectra of 26 reference samples from the substance/substance group *Betamethasone valerate*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Betamethasone valerate	170787	23332	40
Caelo	Betamethasone valerate	172716	23683	40
Caelo	Betamethasone valerate	22001101	26127	38
Caelo	Betamethasone valerate	23002259	26968	40
Euro OTC	Betamethasone valerate	1606023	22716	40
Euro OTC	Betamethasone valerate	1704019	23396	40
Euro OTC	Betamethasone valerate	1801024	23967	40
Euro OTC	Betamethasone valerate	1911001	24982	40
Euro OTC	Betamethasone valerate	2102010	25540	40
Euro OTC	Betamethasone valerate	2202016	26035	40
Euro OTC	Betamethasone valerate	2309023	27009	30
Fagron	Betamethasone valerate	21K09-B05-217898	26171	40
Caelo	Betamethasone valerate	13225507	21588†	6
Caelo	Betamethasone valerate	170787	23332SI	20
Caelo	Betamethasone valerate	172716	23683SI	20
Caelo	Betamethasone valerate	22001101	26127SI	30
Caelo	Betamethasone valerate	23002259	26968SI	34
Euro OTC	Betamethasone valerate	1606023	22716SI	34
Euro OTC	Betamethasone valerate	1610010	22861SI†	30
Euro OTC	Betamethasone valerate	1704019	23396SI	29
Euro OTC	Betamethasone valerate	1801024	23967SI	40
Euro OTC	Betamethasone valerate	1911001	24982SI	40
Euro OTC	Betamethasone valerate	2102010	25540SI	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Betamethasone valerate	2202016	26035SI	10
Euro OTC	Betamethasone valerate	2309023	27009SI	40
Fagron	Betamethasone valerate	21K09-B05-217898	26171SI	40

- 201 203 spectra from a total of 4031 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5621 spectra from 1248 *Apo-Ident* customers from 861 batches from the substance/substance group *Betamethasone valerate*.
- Among them are spectra of independent samples from 805 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Betamethasone valerate		1
	Betamethasone valerate	1208014-04	1
	Betamethasone valerate	181108-01	1
	Betamethasone valerate	21000036021	3
	Betamethasone valerate	21K09-B05-217891	1
	Betamethasone valerate	21K09-B05-217898	1
	Betamethasone valerate	21K09-B05-22018	1
	Betamethasone valerate	21K09-B05-220180	1
	Betamethasone valerate	21K09-B05-220365	1
	Betamethasone valerate	21k09-B05-222192	1
	Betamethasone valerate	21K09-B05-222192	8
	Betamethasone valerate	21K09-B05-222194	1
	Betamethasone valerate	2200101016	1
	Betamethasone valerate	22001101003	7
	Betamethasone valerate	22001101004	1
	Betamethasone valerate	22001101008	4
	Betamethasone valerate	22001101009	3
	Betamethasone valerate	22001101014	1
	Betamethasone valerate	22001101015	10
	Betamethasone valerate	22001101016	9
	Betamethasone valerate	22001101017	4
	Betamethasone valerate	22001101018	11
	Betamethasone valerate	22001101020	11
	Betamethasone valerate	22001101021	5
	Betamethasone valerate	22001101025	2
	Betamethasone valerate	22001102021	1
	Betamethasone valerate	2202015-51	1
	Betamethasone valerate	2202016-01	10
	Betamethasone valerate	2202016-02	6
	Betamethasone valerate	221101020	1
	Betamethasone valerate	22H25-B07-223527	6
	Betamethasone valerate	22H25-B07-227236	2

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Betamethasone valerate	22H25-B07-227293	1
	Betamethasone valerate	22HB07223527	1
	Betamethasone valerate	22K07-B08-227496	1
	Betamethasone valerate	22K07B08229283	1
	Betamethasone valerate	22K07-B08-229283	2
	Betamethasone valerate	23003252001	1
	Betamethasone valerate	23003252003	1
	Betamethasone valerate	2309023-01	10
	Betamethasone valerate	B07-2272306	1
	Betamethasone valerate	BV005/1221	1
/Sanacorp	Betamethasone valerate	17078701	1
03110031	Betamethasone valerate	17271603	1
A.H.D.	Betamethasone valerate	13D03-N07	1
Aep	Betamethasone valerate	22001101018	1
AEP	Betamethasone valerate	F02-3737908	1
agron/Krieger	Betamethasone valerate	12B2B-N01	1
AHC 01.07.13 EK 48,05	Betamethasone valerate	12K07-N23	1
AHD 04.10.17 E.k:18,47	Betamethasone valerate	16270514	1
AHD 15.06.16 EK:18,44	Betamethasone valerate	15398505	1
AHD 17.11.14 EK 18,11	Betamethasone valerate	13091205	1
AHD/Euro	Betamethasone valerate	181100801	1
AHD/Fargon	Betamethasone valerate	14H28-Bo1-302865	1
AHD	Betamethasone valerate	1406019-02	2
AHD	Betamethasone valerate	15262607	1
AHD	Betamethasone valerate	15398515	1
AHD	Betamethasone valerate	17078714	1
AHD	Betamethasone valerate	18199902	1
AHD	Betamethasone valerate	22001101015	1
AHDE / Cael 17.02.2015	Betamethasone valerate	13225516	1
AHL	Betamethasone valerate	15398501	1
ALH	Betamethasone valerate	15398512	1
Alliance Haelthcare	Betamethasone valerate	21K09-B05-220180	1
Alliance Health 06.0...	Betamethasone valerate	13091207	1
Alliance healthcare	Betamethasone valerate	13D03-N07	1
Alliance Healthcare	Betamethasone valerate	1610010-01	1
Alliance/EurRho	Betamethasone valerate	1912012-01	1
Alliance	Betamethasone valerate	22001101017	1
alliance	Betamethasone valerate	2202016-01	1
Allianz Healthcare 2...	Betamethasone valerate	15075802	1
Anzag	Betamethasone valerate	12L11-N01	1
Anzag	Betamethasone valerate	1819908	1
Anzag	Betamethasone valerate	21000036003	2
Audor Pharma	Betamethasone valerate	APBV010/0516B	5
Biomed / Gehe	Betamethasone valerate	1510037-01	1
Bombastus	Betamethasone valerate	12L11-N01	1
Bombastus	Betamethasone valerate	1510037-01	1
Bombastus	Betamethasone valerate	1704019-01	4
Bombatus	Betamethasone valerate	1801024-01	3
Cael Sanacorp 05.02.2016	Betamethasone valerate	14H28-B01-302864	1
Caello/Sanacorp	Betamethasone valerate	15075803	1
Caelo	Betamethasone valerate		3
Caelo	Betamethasone valerate	10296701	1
Caelo	Betamethasone valerate	10296705	2
Caelo	Betamethasone valerate	10296707	1
Caelo	Betamethasone valerate	1108045-03	4
Caelo	Betamethasone valerate	1113	1
Caelo	Betamethasone valerate	11131905	1
Caelo	Betamethasone valerate	11131909	1
Caelo	Betamethasone valerate	11131914	1
Caelo	Betamethasone valerate	11131917	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Betamethasone valerate	1131914	1
Caelo	Betamethasone valerate	1199932	1
Caelo	Betamethasone valerate	12003402	1
Caelo	Betamethasone valerate	12003403	7
Caelo	Betamethasone valerate	12003404	1
Caelo	Betamethasone valerate	12003405	8
Caelo	Betamethasone valerate	12003406	6
Caelo	Betamethasone valerate	12003407	1
Caelo	Betamethasone valerate	12003409	1
Caelo	Betamethasone valerate	12003410	1
Caelo	Betamethasone valerate	12003411	3
Caelo	Betamethasone valerate	1208014-01	1
Caelo	Betamethasone valerate	1208014-03	1
Caelo	Betamethasone valerate	12207004	1
Caelo	Betamethasone valerate	12229802	3
Caelo	Betamethasone valerate	12229804	4
Caelo	Betamethasone valerate	12229805	9
Caelo	Betamethasone valerate	12229806	6
Caelo	Betamethasone valerate	12229808	12
Caelo	Betamethasone valerate	12229809	2
Caelo	Betamethasone valerate	12229810	4
Caelo	Betamethasone valerate	12229811	7
Caelo	Betamethasone valerate	12229812	9
Caelo	Betamethasone valerate	12229813	2
Caelo	Betamethasone valerate	123345	1
Caelo	Betamethasone valerate	129711-5471	1
Caelo	Betamethasone valerate	12B28-N01	1
Caelo	Betamethasone valerate	12g09-n07	1
Caelo	Betamethasone valerate	12G09-N07	3
Caelo	Betamethasone valerate	12K07-N23	1
Caelo	Betamethasone valerate	12L11-N01	1
Caelo	Betamethasone valerate	13012015C	1
Caelo	Betamethasone valerate	13091201	2
Caelo	Betamethasone valerate	13091203	12
Caelo	Betamethasone valerate	13091204	4
Caelo	Betamethasone valerate	13091205	11
Caelo	Betamethasone valerate	13091206	1
Caelo	Betamethasone valerate	13091207	8
Caelo	Betamethasone valerate	13091209	4
Caelo	Betamethasone valerate	13091210	3
Caelo	Betamethasone valerate	13091211	3
Caelo	Betamethasone valerate	13091212	6
Caelo	Betamethasone valerate	13091213	6
Caelo	Betamethasone valerate	13225502	2
Caelo	Betamethasone valerate	13225503	9
Caelo	Betamethasone valerate	13225504	9
Caelo	Betamethasone valerate	13225505	12
Caelo	Betamethasone valerate	13225507	2
Caelo	Betamethasone valerate	13225508	9
Caelo	Betamethasone valerate	13225509	2
Caelo	Betamethasone valerate	13225515	9
Caelo	Betamethasone valerate	13225516	10
Caelo	Betamethasone valerate	13225607	1
Caelo	Betamethasone valerate	13923	1
Caelo	Betamethasone valerate	13D03-N07	3
Caelo	Betamethasone valerate	13G19-N01	1
Caelo	Betamethasone valerate	13K05_B08_292652	1
Caelo	Betamethasone valerate	13K29-B32-288247	1
Caelo	Betamethasone valerate	14031407	1
Caelo	Betamethasone valerate	1406019-01	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Betamethasone valerate	1406019-02	3
Caelo	Betamethasone valerate	140601903	1
Caelo	Betamethasone valerate	1406019-03	4
Caelo	Betamethasone valerate	14188602	2
Caelo	Betamethasone valerate	14188603	5
Caelo	Betamethasone valerate	14188604	8
Caelo	Betamethasone valerate	14188605	1
Caelo	Betamethasone valerate	14188606	1
Caelo	Betamethasone valerate	14188608	8
Caelo	Betamethasone valerate	14188609	5
Caelo	Betamethasone valerate	14188610	7
Caelo	Betamethasone valerate	14188617	3
Caelo	Betamethasone valerate	14188619	3
Caelo	Betamethasone valerate	1488609	1
Caelo	Betamethasone valerate	1488610	1
Caelo	Betamethasone valerate	14C19-B02-292653	1
Caelo	Betamethasone valerate	14G30-B05	1
Caelo	Betamethasone valerate	14G30-B05-309520	1
Caelo	Betamethasone valerate	14H28-B01-302865	1
Caelo	Betamethasone valerate	15/16-B07-317416	1
Caelo	Betamethasone valerate	15/16-B07-317417	1
Caelo	Betamethasone valerate	15/16-B07-319228	2
Caelo	Betamethasone valerate	15075802	22
Caelo	Betamethasone valerate	150758022	1
Caelo	Betamethasone valerate	15075803	9
Caelo	Betamethasone valerate	150758036	1
Caelo	Betamethasone valerate	15075804	8
Caelo	Betamethasone valerate	15075805	8
Caelo	Betamethasone valerate	15075809	4
Caelo	Betamethasone valerate	15075810	9
Caelo	Betamethasone valerate	15075811	1
Caelo	Betamethasone valerate	15075812	3
Caelo	Betamethasone valerate	1510037-01	2
Caelo	Betamethasone valerate	1516-B07-319228	1
Caelo	Betamethasone valerate	1526213	1
Caelo	Betamethasone valerate	15262602	8
Caelo	Betamethasone valerate	15262603	15
Caelo	Betamethasone valerate	15262604	14
Caelo	Betamethasone valerate	15262606	4
Caelo	Betamethasone valerate	15262607	7
Caelo	Betamethasone valerate	15262609	3
Caelo	Betamethasone valerate	15262610	4
Caelo	Betamethasone valerate	15262612	1
Caelo	Betamethasone valerate	15262613	1
Caelo	Betamethasone valerate	1526604	1
Caelo	Betamethasone valerate	1538506	1
Caelo	Betamethasone valerate	15395512	1
Caelo	Betamethasone valerate	15398501	23
Caelo	Betamethasone valerate	15398502	1
Caelo	Betamethasone valerate	15398503	2
Caelo	Betamethasone valerate	15398504	3
Caelo	Betamethasone valerate	15398505	17
Caelo	Betamethasone valerate	15398506	30
Caelo	Betamethasone valerate	15398512	22
Caelo	Betamethasone valerate	15398513	4
Caelo	Betamethasone valerate	15398514	3
Caelo	Betamethasone valerate	15398515	27
Caelo	Betamethasone valerate	15B24-B04	1
Caelo	Betamethasone valerate	15B24-B04-307016	1
Caelo	Betamethasone valerate	15F16-B04-314054	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Betamethasone valerate	15F16-B04-315327	1
Caelo	Betamethasone valerate	15L21-B03-318663	1
Caelo	Betamethasone valerate	160216BV	1
Caelo	Betamethasone valerate	160501	1
Caelo	Betamethasone valerate	160503	1
Caelo	Betamethasone valerate	1606023-01	4
Caelo	Betamethasone valerate	1610010-01	5
Caelo	Betamethasone valerate	161125BV/15398512	1
Caelo	Betamethasone valerate	16270501	17
Caelo	Betamethasone valerate	16270502	37
Caelo	Betamethasone valerate	16270503	18
Caelo	Betamethasone valerate	16270504	1
Caelo	Betamethasone valerate	16270505	16
Caelo	Betamethasone valerate	16270508	2
Caelo	Betamethasone valerate	16270509	9
Caelo	Betamethasone valerate	1627051	1
Caelo	Betamethasone valerate	16270511	26
Caelo	Betamethasone valerate	16270513	22
Caelo	Betamethasone valerate	16270514	9
Caelo	Betamethasone valerate	16720513	1
Caelo	Betamethasone valerate	16B18-B02-320971	2
Caelo	Betamethasone valerate	16B18-B02-322121	2
Caelo	Betamethasone valerate	16B18-B02-324798	1
Caelo	Betamethasone valerate	16E23-B03	1
Caelo	Betamethasone valerate	16E23-B03-324799	2
Caelo	Betamethasone valerate	16E23-B03-324800	1
Caelo	Betamethasone valerate	16e23-b03-328128	1
Caelo	Betamethasone valerate	16E23-B03-328128	3
Caelo	Betamethasone valerate	16H22-B06-331273	1
Caelo	Betamethasone valerate	16H22B06332351	1
Caelo	Betamethasone valerate	16H22-B06-332351	1
Caelo	Betamethasone valerate	17/251/Bv	1
Caelo	Betamethasone valerate	170401901	4
Caelo	Betamethasone valerate	1704019-01	18
Caelo	Betamethasone valerate	17078103	1
Caelo	Betamethasone valerate	1707814	1
Caelo	Betamethasone valerate	1707815	2
Caelo	Betamethasone valerate	1707819	1
Caelo	Betamethasone valerate	17078701	25
Caelo	Betamethasone valerate	17078702	1
Caelo	Betamethasone valerate	17078703	35
Caelo	Betamethasone valerate	17078704	7
Caelo	Betamethasone valerate	17078705	1
Caelo	Betamethasone valerate	17078707	1
Caelo	Betamethasone valerate	17078711	7
Caelo	Betamethasone valerate	17078712	13
Caelo	Betamethasone valerate	17078713	19
Caelo	Betamethasone valerate	17078714	17
Caelo	Betamethasone valerate	17078715	16
Caelo	Betamethasone valerate	17078716	1
Caelo	Betamethasone valerate	17078719	18
Caelo	Betamethasone valerate	17078720	25
Caelo	Betamethasone valerate	1708701	1
Caelo	Betamethasone valerate	17196001	1
Caelo	Betamethasone valerate	17271601	7
Caelo	Betamethasone valerate	17271602	1
Caelo	Betamethasone valerate	17271603	29
Caelo	Betamethasone valerate	17271604	9
Caelo	Betamethasone valerate	1729002	1
Caelo	Betamethasone valerate	17329001	29

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Betamethasone valerate	17329002	39
Caelo	Betamethasone valerate	17329003	17
Caelo	Betamethasone valerate	17329004	6
Caelo	Betamethasone valerate	17329008	10
Caelo	Betamethasone valerate	17329011	7
Caelo	Betamethasone valerate	17329015	15
Caelo	Betamethasone valerate	17329017	10
Caelo	Betamethasone valerate	17329018	76
Caelo	Betamethasone valerate	1732901803110025	1
Caelo	Betamethasone valerate	17329019	4
Caelo	Betamethasone valerate	173296011	1
Caelo	Betamethasone valerate	1739002	3
Caelo	Betamethasone valerate	17C29-B04	2
Caelo	Betamethasone valerate	17C29-B04-334329	1
Caelo	Betamethasone valerate	17C29-B04-335676	2
Caelo	Betamethasone valerate	17G31B04338575	1
Caelo	Betamethasone valerate	17G31-B04-338575	1
Caelo	Betamethasone valerate	17G31-B04-341576	1
Caelo	Betamethasone valerate	17K16-B0/8-347310	1
Caelo	Betamethasone valerate	17K16-B08	1
Caelo	Betamethasone valerate	17K16-B08-345541	3
Caelo	Betamethasone valerate	17K16-B08-347309	2
Caelo	Betamethasone valerate	17K16-B08-347912	1
Caelo	Betamethasone valerate	1801024-01	12
Caelo	Betamethasone valerate	18071403	1
Caelo	Betamethasone valerate	1811008	1
Caelo	Betamethasone valerate	181100801	1
Caelo	Betamethasone valerate	1811008-01	3
Caelo	Betamethasone valerate	18121206	1
Caelo	Betamethasone valerate	18189907	1
Caelo	Betamethasone valerate	1819908	1
Caelo	Betamethasone valerate	1819918	3
Caelo	Betamethasone valerate	1819924	1
Caelo	Betamethasone valerate	1819932	1
Caelo	Betamethasone valerate	181999007	1
Caelo	Betamethasone valerate	18199902	43
Caelo	Betamethasone valerate	18199903	2
Caelo	Betamethasone valerate	18199906	10
Caelo	Betamethasone valerate	18199907	37
Caelo	Betamethasone valerate	1819990705/2023	1
Caelo	Betamethasone valerate	18199908	15
Caelo	Betamethasone valerate	18199914	4
Caelo	Betamethasone valerate	18199915	4
Caelo	Betamethasone valerate	18199916	21
Caelo	Betamethasone valerate	18199918	50
Caelo	Betamethasone valerate	18199923P-200116-2	1
Caelo	Betamethasone valerate	18199924	19
Caelo	Betamethasone valerate	18199926	4
Caelo	Betamethasone valerate	18199930	8
Caelo	Betamethasone valerate	18199932	46
Caelo	Betamethasone valerate	18199933	36
Caelo	Betamethasone valerate	18199937	2
Caelo	Betamethasone valerate	18199938	8
Caelo	Betamethasone valerate	18G03-B03-351731	1
Caelo	Betamethasone valerate	18I27-B05-354880	1
Caelo	Betamethasone valerate	1912012-01	2
Caelo	Betamethasone valerate	19220009	1
Caelo	Betamethasone valerate	1922070003	1
Caelo	Betamethasone valerate	192207001	18
Caelo	Betamethasone valerate	192207002	42

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Betamethasone valerate	192207003	32
Caelo	Betamethasone valerate	192207004	4
Caelo	Betamethasone valerate	192207006	11
Caelo	Betamethasone valerate	192207009	27
Caelo	Betamethasone valerate	192207010	20
Caelo	Betamethasone valerate	192207012	21
Caelo	Betamethasone valerate	19220702	34
Caelo	Betamethasone valerate	19220703	7
Caelo	Betamethasone valerate	19220704	26
Caelo	Betamethasone valerate	19220705	42
Caelo	Betamethasone valerate	19220706	1
Caelo	Betamethasone valerate	19220707012	1
Caelo	Betamethasone valerate	19g30-b02-363673	1
Caelo	Betamethasone valerate	19g30-b02-363693	1
Caelo	Betamethasone valerate	20002685001	6
Caelo	Betamethasone valerate	20B18-F07-370009	2
Caelo	Betamethasone valerate	20B18-F07-370010	1
Caelo	Betamethasone valerate	21000026003	2
Caelo	Betamethasone valerate	210000360010	2
Caelo	Betamethasone valerate	21000036003	58
Caelo	Betamethasone valerate	21000036004	22
Caelo	Betamethasone valerate	210000360063	1
Caelo	Betamethasone valerate	21000036007	2
Caelo	Betamethasone valerate	21000036008	11
Caelo	Betamethasone valerate	21000036010	32
Caelo	Betamethasone valerate	21000036011	1
Caelo	Betamethasone valerate	21000036013	1
Caelo	Betamethasone valerate	21000036016	19
Caelo	Betamethasone valerate	21000036017	39
Caelo	Betamethasone valerate	21000036018	2
Caelo	Betamethasone valerate	21000036019	1
Caelo	Betamethasone valerate	21000036020	19
Caelo	Betamethasone valerate	21000036021	19
Caelo	Betamethasone valerate	21000036022	2
Caelo	Betamethasone valerate	2100003610	1
Caelo	Betamethasone valerate	2100036003	4
Caelo	Betamethasone valerate	2100036004	1
Caelo	Betamethasone valerate	2100036010	2
Caelo	Betamethasone valerate	2100036016	1
Caelo	Betamethasone valerate	2100036020	1
Caelo	Betamethasone valerate	2100036021	1
Caelo	Betamethasone valerate	210003610	1
Caelo	Betamethasone valerate	210112	1
Caelo	Betamethasone valerate	210201001	1
Caelo	Betamethasone valerate	2102010-02	1
Caelo	Betamethasone valerate	21G28-B02-213516	1
Caelo	Betamethasone valerate	22001101002	2
Caelo	Betamethasone valerate	22001101003	1
Caelo	Betamethasone valerate	22001101004	3
Caelo	Betamethasone valerate	22001101005	16
Caelo	Betamethasone valerate	22001101009	5
Caelo	Betamethasone valerate	22001101015	2
Caelo	Betamethasone valerate	22001101016	2
Caelo	Betamethasone valerate	22001101018	1
Caelo	Betamethasone valerate	2x12229813	1
Caelo	Betamethasone valerate	31(17329018)	1
Caelo	Betamethasone valerate	311002517078712	1
Caelo	Betamethasone valerate	3303	1
Caelo	Betamethasone valerate	534210000363	1
Caelo	Betamethasone valerate	8081502	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Betamethasone valerate	922070101	1
Caelo	Betamethasone valerate	APPV010/0516B	1
Caelo	Betamethasone valerate	B03041205	1
Caelo	Betamethasone valerate	BV018/0715	2
Caelo	Betamethasone valerate	BV109/0519	1
Caelo	Betamethasone valerate	BV-BLT225/0514	1
Caelo	Betamethasone valerate	F07-3667709	1
Caelo	Betamethasone valerate	NT0597M	1
Caeolo /Sana	Betamethasone valerate	18199903	1
Caesar & Lorenz GmbH	Betamethasone valerate	15075805	1
Caesar & Lorenz GmbH	Betamethasone valerate	16270501	1
Caesar & Loretz GmbH...	Betamethasone valerate	21000036020	1
Caesar & Loretz GmbH...	Betamethasone valerate	19220702	1
Caesar & Loretz GmbH...	Betamethasone valerate	21000036004	1
Caesar & Loretz GmbH...	Betamethasone valerate	18199938	1
Caesar & Loretz GmbH...	Betamethasone valerate	22001101005	1
Caesar & Loretz GmbH...	Betamethasone valerate	21000036011	1
Caesar & Loretz GmbH...	Betamethasone valerate	120801402	1
Caesar & Loretz GmbH...	Betamethasone valerate	10296707	1
Caesar & Loretz GmbH...	Betamethasone valerate	12003404	1
Caesar & Loretz GmbH...	Betamethasone valerate	12003409	2
Caesar & Loretz GmbH...	Betamethasone valerate	12229809	1
Caesar & Loretz GmbH...	Betamethasone valerate	13091206	2
Caesar & Loretz GmbH...	Betamethasone valerate	13091211	1
Caesar & Loretz GmbH...	Betamethasone valerate	21000036008	1
Caesar & Loretz GmbH...	Betamethasone valerate	22001101005	1
Caesar & Loretz GmbH...	Betamethasone valerate	18199915	1
Caesar & Loretz GmbH...	Betamethasone valerate	22001101015	1
Caesar & Loretz GmbH...	Betamethasone valerate	18199916	1
Caesar & Loretz GmbH...	Betamethasone valerate	22001101009	1
Caesar & Loretz GmbH...	Betamethasone valerate	22001101005	1
Caesar & Loretz GmbH...	Betamethasone valerate	18199902	1
Caesar & Loretz GmbH/	Betamethasone valerate	17329018	1
Caesar & Loretz GmbH/AEP	Betamethasone valerate	18199924	1
Caesar & Loretz GmbH/E	Betamethasone valerate	18199938	1
Caesar & Loretz GmbH/E	Betamethasone valerate	21000036016	1
Caesar & Loretz GmbH...	Betamethasone valerate	20002685001	2
Caesar & Loretz GmbH/Gehe	Betamethasone valerate	18199903	1
Caesar & Loretz GmbH/Gehe	Betamethasone valerate	18199908	1
Caesar & Loretz GmbH/Gehe	Betamethasone valerate	18199916	1
Caesar & Loretz GmbH/Gehe	Betamethasone valerate	19220702	1
Caesar & Loretz GmbH/Gehe	Betamethasone valerate	21000036010	1
Caesar & Loretz GmbH/Gehe	Betamethasone valerate	21000036016	1
Caesar & Loretz GmbH/Gehe	Betamethasone valerate	22001101021	1
Caesar & Loretz GmbH...	Betamethasone valerate	21000036010	1
Caesar & Loretz GmbH/Gö	Betamethasone valerate	21000036021	2
Caesar & Loretz GmbH...	Betamethasone valerate	18199918	1
Caesar & Loretz GmbH...	Betamethasone valerate	21000036003	3
Caesar & Loretz GmbH...	Betamethasone valerate	192207010	1
Caesar & Loretz GmbH...	Betamethasone valerate	18199918	1
Caesar & Loretz GmbH...	Betamethasone valerate	18199933	1
Caesar & Loretz GmbH...	Betamethasone valerate	192207010	1
Caesar & Loretz GmbH...	Betamethasone valerate	19220705	1
Caesar & Loretz GmbH...	Betamethasone valerate	21000036016	1
Caesar & Loretz GmbH...	Betamethasone valerate	22001101004	1
Caesar & Loretz GmbH...	Betamethasone valerate	22001101015	1
Caesar & Loretz GmbH/K	Betamethasone valerate	19220702	1
Caesar & Loretz GmbH/Kehr	Betamethasone valerate	21000036021	1
Caesar & Loretz GmbH...	Betamethasone valerate	18199918	1
Caesar & Loretz GmbH...	Betamethasone valerate	21000036010	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Betamethasone valerate	18199907	1
Caesar & Loretz GmbH...	Betamethasone valerate	18199908	1
Caesar & Loretz GmbH...	Betamethasone valerate	18199918	1
Caesar & Loretz GmbH...	Betamethasone valerate	18199933	1
Caesar & Loretz GmbH...	Betamethasone valerate	192207002	1
Caesar & Loretz GmbH...	Betamethasone valerate	192207010	2
Caesar & Loretz GmbH...	Betamethasone valerate	21000036003	3
Caesar & Loretz GmbH...	Betamethasone valerate	21000036010	1
Caesar & Loretz GmbH...	Betamethasone valerate	21000036021	1
Caesar & Loretz GmbH...	Betamethasone valerate	18199915	1
Caesar & Loretz GmbH...	Betamethasone valerate	18199924	2
Caesar & Loretz GmbH...	Betamethasone valerate	18G03-B03-352460	1
Caesar & Loretz GmbH...	Betamethasone valerate	19220704	2
Caesar & Loretz GmbH...	Betamethasone valerate	20002685001	1
Caesar & Loretz GmbH...	Betamethasone valerate	21000036003	2
Caesar & Loretz GmbH...	Betamethasone valerate	21000036004	1
Caesar & Loretz GmbH...	Betamethasone valerate	BV116/0819	1
Caesar & Loretz GmbH...	Betamethasone valerate	18199918	1
Caesar & Loretz GmbH...	Betamethasone valerate	21000036017	2
Caesar & Loretz GmbH...	Betamethasone valerate	192207002	1
Caesar & Loretz GmbH...	Betamethasone valerate	192207009	3
Caesar & Loretz GmbH...	Betamethasone valerate	19220705	1
Caesar & Loretz GmbH...	Betamethasone valerate	21000036003	2
Caesar & Loretz GmbH...	Betamethasone valerate	22001101005	1
Caesar & Loretz GmbH...	Betamethasone valerate	22001101015	1
Caesar & Loretz GmbH...	Betamethasone valerate	18199915	1
Caesar & Loretz GmbH...	Betamethasone valerate	18199932	2
Caesar & Loretz GmbH...	Betamethasone valerate	19220702	1
Caesar & Loretz GmbH...	Betamethasone valerate	19220703	1
Caesar & Loretz GmbH...	Betamethasone valerate	21000036004	2
Caesar & Loretz GmbH...	Betamethasone valerate	21000036017	1
Caesar & Loretz GmbH	Betamethasone valerate	13225504	1
Caesar & Loretz GmbH	Betamethasone valerate	16270511	1
Caesar & Loretz GmbH	Betamethasone valerate	17078701	1
Caesar & Loretz GmbH	Betamethasone valerate	17329001	1
Caesar & Loretz GmbH	Betamethasone valerate	17329002	1
Caesar & Loretz GmbH	Betamethasone valerate	17329004	1
Caesar & Loretz GmbH	Betamethasone valerate	17329015	1
Caesar & Loretz GmbH	Betamethasone valerate	17329018	5
Caesar & Loretz GmbH	Betamethasone valerate	17K16B08345555	1
Caesar & Loretz GmbH	Betamethasone valerate	1811008-01	2
Caesar & Loretz GmbH	Betamethasone valerate	1819930	1
Caesar & Loretz GmbH	Betamethasone valerate	18199902	1
Caesar & Loretz GmbH	Betamethasone valerate	18199903	1
Caesar & Loretz GmbH	Betamethasone valerate	18199906	1
Caesar & Loretz GmbH	Betamethasone valerate	18199907	8
Caesar & Loretz GmbH	Betamethasone valerate	18199908	3
Caesar & Loretz GmbH	Betamethasone valerate	18199914	1
Caesar & Loretz GmbH	Betamethasone valerate	18199915	4
Caesar & Loretz GmbH	Betamethasone valerate	18199916	3
Caesar & Loretz GmbH	Betamethasone valerate	18199918	15
Caesar & Loretz GmbH	Betamethasone valerate	18199923	1
Caesar & Loretz GmbH	Betamethasone valerate	18199924	6
Caesar & Loretz GmbH	Betamethasone valerate	18199930	1
Caesar & Loretz GmbH	Betamethasone valerate	18199932	7
Caesar & Loretz GmbH	Betamethasone valerate	18199933	11
Caesar & Loretz GmbH	Betamethasone valerate	18199937	1
Caesar & Loretz GmbH	Betamethasone valerate	18199938	5
Caesar & Loretz GmbH	Betamethasone valerate	18G03-B03	1
Caesar & Loretz GmbH	Betamethasone valerate	192207001	8

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Betamethasone valerate	192207002	12
Caesar & Loretz GmbH	Betamethasone valerate	192207003	8
Caesar & Loretz GmbH	Betamethasone valerate	192207004	1
Caesar & Loretz GmbH	Betamethasone valerate	192207005	1
Caesar & Loretz GmbH	Betamethasone valerate	192207006	1
Caesar & Loretz GmbH	Betamethasone valerate	192207009	5
Caesar & Loretz GmbH	Betamethasone valerate	192207010	7
Caesar & Loretz GmbH	Betamethasone valerate	192207012	11
Caesar & Loretz GmbH	Betamethasone valerate	19220702	12
Caesar & Loretz GmbH	Betamethasone valerate	19220703	1
Caesar & Loretz GmbH	Betamethasone valerate	19220704	11
Caesar & Loretz GmbH	Betamethasone valerate	19220705	3
Caesar & Loretz GmbH	Betamethasone valerate	19220706	1
Caesar & Loretz GmbH	Betamethasone valerate	19220707	1
Caesar & Loretz GmbH	Betamethasone valerate	1922207002	1
Caesar & Loretz GmbH	Betamethasone valerate	21000036001	1
Caesar & Loretz GmbH	Betamethasone valerate	21000036003	16
Caesar & Loretz GmbH	Betamethasone valerate	21000036004	13
Caesar & Loretz GmbH	Betamethasone valerate	21000036007	2
Caesar & Loretz GmbH	Betamethasone valerate	21000036008	6
Caesar & Loretz GmbH	Betamethasone valerate	21000036010	8
Caesar & Loretz GmbH	Betamethasone valerate	21000036011	1
Caesar & Loretz GmbH	Betamethasone valerate	21000036015	1
Caesar & Loretz GmbH	Betamethasone valerate	21000036016	12
Caesar & Loretz GmbH	Betamethasone valerate	21000036017	13
Caesar & Loretz GmbH	Betamethasone valerate	21000036018	1
Caesar & Loretz GmbH	Betamethasone valerate	21000036019	3
Caesar & Loretz GmbH	Betamethasone valerate	21000036020	8
Caesar & Loretz GmbH	Betamethasone valerate	21000036021	7
Caesar & Loretz GmbH	Betamethasone valerate	21000036023	1
Caesar & Loretz GmbH	Betamethasone valerate	22001101002	1
Caesar & Loretz GmbH	Betamethasone valerate	22001101004	2
Caesar & Loretz GmbH	Betamethasone valerate	22001101005	2
Caesar & Loretz GmbH	Betamethasone valerate	22001101009	3
Caesar & Loretz GmbH	Betamethasone valerate	22001101015	2
Caesar & Loretz GmbH	Betamethasone valerate	22001101016	1
Caesar & Loretz GmbH	Betamethasone valerate	22001101023	2
Caesar & Loretz/Gehe	Betamethasone valerate	18199932	1
Caesar & Loretz/Geil...	Betamethasone valerate	192207001	1
Caesar & Loretz	Betamethasone valerate	17329016	1
Caesar & Loretz	Betamethasone valerate	21000036008	1
Caesar &Loretz GmbH	Betamethasone valerate	11131917	1
Caesar Loretz	Betamethasone valerate	192207010	1
Caesar und Loretz	Betamethasone valerate	15075803	1
Caesar&Lorenz	Betamethasone valerate	21000036016	1
Caesar&Loretz GmbH,P...	Betamethasone valerate	16270509	1
Caesar&Loretz GmbH/Anzag	Betamethasone valerate	15075802	1
Caesar&Loretz GmbH	Betamethasone valerate	15262609	1
caesar&loretz,phönix	Betamethasone valerate	14188606	1
Caesar/Lorenz	Betamethasone valerate	12003403	1
Caleo/Phönix	Betamethasone valerate	1522609	1
Carlo/Gehe	Betamethasone valerate	19220702	1
Carlo/Phönix/46,64	Betamethasone valerate	18199924	1
Cealo/Gehe	Betamethasone valerate	17329002	1
Cealo/Gehe	Betamethasone valerate	1739002	1
Cealo/Gehe	Betamethasone valerate	1801024-01	1
Cealo/Noweda	Betamethasone valerate	16270509	2
Cealo	Betamethasone valerate	17078716	1
Crystal PH/Oberlinde...	Betamethasone valerate	C0073/114040	1
Dr. Aug. Wolff GmbH ...	Betamethasone valerate	192207012	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
E Plus	Betamethasone valerate	16270502	1
E Plus	Betamethasone valerate	17329002	1
Ebert & Jacobi	Betamethasone valerate	14188606	1
Ebert & Jacobi	Betamethasone valerate	15075810	1
Ebert u. Jacobi 1...	Betamethasone valerate	15/16-B07-317417	1
Eigenherstellung	Betamethasone valerate	9070313	1
EuRho / Phoenix	Betamethasone valerate	1704019-01	1
EuRho /Gumo	Betamethasone valerate	1911001-01	1
EuRho/Noweda 02.06.2022	Betamethasone valerate	2102010	1
EuRho/Noweda 11.11.2020	Betamethasone valerate	1912012-01	1
EuRho/Noweda	Betamethasone valerate	1911001-01	16
EuRho/Phönix	Betamethasone valerate	2102010-01	1
EuRho/Sanacorp	Betamethasone valerate	1911001-01	1
EuRho/Spangro	Betamethasone valerate	1811008-01	2
EuRho	Betamethasone valerate	1208014-01	2
EuRho	Betamethasone valerate	1208014-02	1
EuRho	Betamethasone valerate	1610010-01	2
Eurho	Betamethasone valerate	1801024-01	1
EuRho	Betamethasone valerate	180102401	1
EuRho	Betamethasone valerate	1801024-01	4
EuRho	Betamethasone valerate	181008-01	1
Eurho	Betamethasone valerate	1811008-01	1
Eurho	Betamethasone valerate	1911001-01	1
EuRho	Betamethasone valerate	1911001-01	1
EuRho	Betamethasone valerate	1911001-02	1
EuRho	Betamethasone valerate	1912012-01	1
EuRho	Betamethasone valerate	2102010-01	2
Euro / Gehe	Betamethasone valerate	1912012-12	1
Euro OTC	Betamethasone valerate		1
Euro OTC	Betamethasone valerate	1031707	1
Euro OTC	Betamethasone valerate	110804-02	1
Euro OTC	Betamethasone valerate	1108045-01	2
Euro OTC	Betamethasone valerate	1108045-02	3
Euro OTC	Betamethasone valerate	110804503	1
Euro OTC	Betamethasone valerate	1108045-03	7
Euro OTC	Betamethasone valerate	1206014-02	1
Euro OTC	Betamethasone valerate	1208014-01	12
Euro OTC	Betamethasone valerate	120801402	2
Euro OTC	Betamethasone valerate	1208014-02	12
Euro OTC	Betamethasone valerate	120801403	1
Euro OTC	Betamethasone valerate	1208014-03	4
Euro OTC	Betamethasone valerate	120801404	1
Euro OTC	Betamethasone valerate	1208014-04	4
Euro OTC	Betamethasone valerate	120812-02	1
Euro OTC	Betamethasone valerate	12L11-N01	1
Euro OTC	Betamethasone valerate	1311039	1
Euro OTC	Betamethasone valerate	131103901	1
Euro OTC	Betamethasone valerate	1311039-01	22
Euro OTC	Betamethasone valerate	131139-01	1
Euro OTC	Betamethasone valerate	13D03-N07	1
Euro OTC	Betamethasone valerate	13K29-B32-289364	1
Euro OTC	Betamethasone valerate	1406011903	1
Euro OTC	Betamethasone valerate	140601901	1
Euro OTC	Betamethasone valerate	1406019-01	25
Euro OTC	Betamethasone valerate	140601902	1
Euro OTC	Betamethasone valerate	1406019-02	23
Euro OTC	Betamethasone valerate	140601903	2
Euro OTC	Betamethasone valerate	1406019-03	32
Euro OTC	Betamethasone valerate	14C19-B02-292650	2
Euro OTC	Betamethasone valerate	15/16-B07-319228	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Betamethasone valerate	1510037	1
Euro OTC	Betamethasone valerate	151003701	1
Euro OTC	Betamethasone valerate	1510037-01	24
Euro OTC	Betamethasone valerate	1510037-07	1
Euro OTC	Betamethasone valerate	1516B07317416	1
Euro OTC	Betamethasone valerate	15398501	1
Euro OTC	Betamethasone valerate	15F16/B04-314054	1
Euro OTC	Betamethasone valerate	1606023-01	41
Euro OTC	Betamethasone valerate	160623-01	1
Euro OTC	Betamethasone valerate	16100100-01	1
Euro OTC	Betamethasone valerate	161001001	1
Euro OTC	Betamethasone valerate	1610010-01	55
Euro OTC	Betamethasone valerate	1610010-03	1
Euro OTC	Betamethasone valerate	16270505	1
Euro OTC	Betamethasone valerate	16E23-B03-328128	3
Euro OTC	Betamethasone valerate	1704018-01	1
Euro OTC	Betamethasone valerate	1704019	2
Euro OTC	Betamethasone valerate	1704019_01	1
Euro OTC	Betamethasone valerate	1704019-0	1
Euro OTC	Betamethasone valerate	170401901	5
Euro OTC	Betamethasone valerate	1704019-01	140
Euro OTC	Betamethasone valerate	1704019-1	1
Euro OTC	Betamethasone valerate	1704021-04	1
Euro OTC	Betamethasone valerate	170419-01	1
Euro OTC	Betamethasone valerate	17078701	1
Euro OTC	Betamethasone valerate	17078703	1
Euro OTC	Betamethasone valerate	17078720	1
Euro OTC	Betamethasone valerate	17271603	3
Euro OTC	Betamethasone valerate	17329001	1
Euro OTC	Betamethasone valerate	1739002	1
Euro OTC	Betamethasone valerate	1740419-01	1
Euro OTC	Betamethasone valerate	17C29-B04-336434	1
Euro OTC	Betamethasone valerate	17K16-B08-345541	1
Euro OTC	Betamethasone valerate	17o4019-01	1
Euro OTC	Betamethasone valerate	18010024-01	1
Euro OTC	Betamethasone valerate	1801024	1
Euro OTC	Betamethasone valerate	1801024_01	1
Euro OTC	Betamethasone valerate	180102401	2
Euro OTC	Betamethasone valerate	1801024-01	133
Euro OTC	Betamethasone valerate	180104-01	1
Euro OTC	Betamethasone valerate	181008-01	1
Euro OTC	Betamethasone valerate	1811008	1
Euro OTC	Betamethasone valerate	181100801	5
Euro OTC	Betamethasone valerate	1811008-01	124
Euro OTC	Betamethasone valerate	1811008-1	2
Euro OTC	Betamethasone valerate	1811024-01	1
Euro OTC	Betamethasone valerate	18199902	1
Euro OTC	Betamethasone valerate	18199907	1
Euro OTC	Betamethasone valerate	190451504	1
Euro OTC	Betamethasone valerate	191001-01	2
Euro OTC	Betamethasone valerate	191100101	1
Euro OTC	Betamethasone valerate	1911001-01	132
Euro OTC	Betamethasone valerate	1911001-02	6
Euro OTC	Betamethasone valerate	191101-01	1
Euro OTC	Betamethasone valerate	1911011-01	1
Euro OTC	Betamethasone valerate	1912012-01	20
Euro OTC	Betamethasone valerate	2014Q1181	1
Euro OTC	Betamethasone valerate	20906	1
Euro OTC	Betamethasone valerate	2102010	3
Euro OTC	Betamethasone valerate	210201001	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Betamethasone valerate	2102010-01	65
Euro OTC	Betamethasone valerate	2102010-02	21
Euro OTC	Betamethasone valerate	210210-01	1
Euro OTC	Betamethasone valerate	2202016-01	24
Euro OTC	Betamethasone valerate	2507211181	1
Euro OTC	Betamethasone valerate	29061805	1
Euro OTC	Betamethasone valerate	3313U-01181	1
Euro OTC	Betamethasone valerate	7071802	1
Euro OTC	Betamethasone valerate	BV116/1117	1
Euro OTC	Betamethasone valerate	BV-BLT221/0314	1
Euro Pharma/Noweda	Betamethasone valerate	1912012-01	6
euro//Noweda	Betamethasone valerate	1801024-01	2
Euro/Alliance Healthcare	Betamethasone valerate	1510037-01	1
Euro/direkt	Betamethasone valerate	1704019-01	1
Euro/Gehe	Betamethasone valerate	1704019-01	1
Euro/Sanacorp	Betamethasone valerate	1801024-01	2
Euro	Betamethasone valerate	1406019-03	3
Euro	Betamethasone valerate	1801024-01	2
Euroo	Betamethasone valerate	1406019-03	1
Europ Ots Pharma	Betamethasone valerate	12l11-N01	1
EurRho/Gehe	Betamethasone valerate	1610010-01	1
Fagon / Noweda	Betamethasone valerate	21G-28-B02-213663	1
Fagon/Noweda	Betamethasone valerate	F07-3667806	1
Fagron	Betamethasone valerate		3
Fagron	Betamethasone valerate	1018E-01181	1
Fagron	Betamethasone valerate	11A04-N02	1
Fagron	Betamethasone valerate	11E18-N03	3
Fagron	Betamethasone valerate	11K18-N09	2
Fagron	Betamethasone valerate	11K-18-N09	1
Fagron	Betamethasone valerate	120801402	1
Fagron	Betamethasone valerate	123649978B	1
Fagron	Betamethasone valerate	12B28-N01	8
Fagron	Betamethasone valerate	12G09-N07	23
Fagron	Betamethasone valerate	12K07N23	1
Fagron	Betamethasone valerate	12K07-N23	6
Fagron	Betamethasone valerate	12L11-N01	18
Fagron	Betamethasone valerate	12L11-NO1	1
Fagron	Betamethasone valerate	13/17-B08-292649	2
Fagron	Betamethasone valerate	1311039-01	1
Fagron	Betamethasone valerate	13d03-n07	3
Fagron	Betamethasone valerate	13D03-N07	38
Fagron	Betamethasone valerate	13g19-n01	2
Fagron	Betamethasone valerate	13G19N01	1
Fagron	Betamethasone valerate	13G19-N01	49
Fagron	Betamethasone valerate	13G19-NO1	1
Fagron	Betamethasone valerate	13K05-B08	2
Fagron	Betamethasone valerate	13K05-B08-092652	1
Fagron	Betamethasone valerate	13K05-B08-291663	3
Fagron	Betamethasone valerate	13K05-B08-292647	2
Fagron	Betamethasone valerate	13K05-B08-292651	1
Fagron	Betamethasone valerate	13K05-B08-292652	2
Fagron	Betamethasone valerate	13K29-B12-288247	1
Fagron	Betamethasone valerate	13K29-B23-288246	1
Fagron	Betamethasone valerate	13K29B32	1
Fagron	Betamethasone valerate	13K29-B32	6
Fagron	Betamethasone valerate	13K29-B32-28824	1
Fagron	Betamethasone valerate	13K29B32288243	1
Fagron	Betamethasone valerate	13K29-B32-288244	2
Fagron	Betamethasone valerate	13K29-B32-288245	1
Fagron	Betamethasone valerate	13K29-B32-288246	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Betamethasone valerate	13k29b32288247	1
Fagron	Betamethasone valerate	13K29-B32-288247	20
Fagron	Betamethasone valerate	13K29-B32-288248	3
Fagron	Betamethasone valerate	13K29-B32-288250	3
Fagron	Betamethasone valerate	13117-B08-292649	2
Fagron	Betamethasone valerate	1406019-03	1
Fagron	Betamethasone valerate	14188603	1
Fagron	Betamethasone valerate	14C19B02	1
Fagron	Betamethasone valerate	14C19-B02	3
Fagron	Betamethasone valerate	14C19-B02-292646	1
Fagron	Betamethasone valerate	14C19-B02-292648	1
Fagron	Betamethasone valerate	14c19-b02-292650	1
Fagron	Betamethasone valerate	14C19-B02-292650	4
Fagron	Betamethasone valerate	14C19-B02-292653	6
Fagron	Betamethasone valerate	14C19B02296168	1
Fagron	Betamethasone valerate	14C19-B02-296168	4
Fagron	Betamethasone valerate	14c19-b02-296169	1
Fagron	Betamethasone valerate	14C19-B02-296169	1
Fagron	Betamethasone valerate	14G30-B05	4
Fagron	Betamethasone valerate	14G30-B05-29617	1
Fagron	Betamethasone valerate	14G30-B05-296170	1
Fagron	Betamethasone valerate	14G30B05296172	1
Fagron	Betamethasone valerate	14G30-B05-296172	3
Fagron	Betamethasone valerate	14G30-B05-296173	14
Fagron	Betamethasone valerate	14G30-B05-296175	3
Fagron	Betamethasone valerate	14G30-B05-309518	2
Fagron	Betamethasone valerate	14G30B05309519	1
Fagron	Betamethasone valerate	14G30-B05-309519	1
Fagron	Betamethasone valerate	14G30-B05-309520	7
Fagron	Betamethasone valerate	14G30-B05-309521	1
Fagron	Betamethasone valerate	14G30-B05-309528	1
Fagron	Betamethasone valerate	14G30-Bo5-296172	1
Fagron	Betamethasone valerate	14G31-B04-342639	1
Fagron	Betamethasone valerate	14H28B01	1
Fagron	Betamethasone valerate	14H28-B01	3
Fagron	Betamethasone valerate	14H28-B01-302683	1
Fagron	Betamethasone valerate	14H28-B01-302863	5
Fagron	Betamethasone valerate	14H28B01302864	1
Fagron	Betamethasone valerate	14H28-B01-302864	6
Fagron	Betamethasone valerate	14H28-B01-302864/201	1
Fagron	Betamethasone valerate	14h28-b01-302865	2
Fagron	Betamethasone valerate	14H28-B01-302865	13
Fagron	Betamethasone valerate	14H28-b01-302866	1
Fagron	Betamethasone valerate	14H28-B01-302866	7
Fagron	Betamethasone valerate	14H28-B01-302877	3
Fagron	Betamethasone valerate	14H28-B01-305470	2
Fagron	Betamethasone valerate	15/16-B07	1
Fagron	Betamethasone valerate	15/16-B07-317416	5
Fagron	Betamethasone valerate	15/16-B07-317417	2
Fagron	Betamethasone valerate	15/16-B07-317428	3
Fagron	Betamethasone valerate	15/16-B07-319228	3
Fagron	Betamethasone valerate	15/16-B07-319831	1
Fagron	Betamethasone valerate	15/16-B07-319832	1
Fagron	Betamethasone valerate	15075802	1
Fagron	Betamethasone valerate	15116-B07	1
Fagron	Betamethasone valerate	1516-B07-317416	1
Fagron	Betamethasone valerate	1526260	1
Fagron	Betamethasone valerate	15398515	1
Fagron	Betamethasone valerate	15824-B04	1
Fagron	Betamethasone valerate	15B24-B04	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Betamethasone valerate	15B24-B04-307015	4
Fagron	Betamethasone valerate	15B24-B04-307016	14
Fagron	Betamethasone valerate	15F16-804-314054	1
Fagron	Betamethasone valerate	15F16-B04	4
Fagron	Betamethasone valerate	15F16-B04-215327	1
Fagron	Betamethasone valerate	15f16-b04314054	1
Fagron	Betamethasone valerate	15F16-B04-314054	5
Fagron	Betamethasone valerate	15F16-B04-314054/201	1
Fagron	Betamethasone valerate	15F16-B04-314055	1
Fagron	Betamethasone valerate	15F16-B04-314882	1
Fagron	Betamethasone valerate	15F16-B04-315328	3
Fagron	Betamethasone valerate	15I16-B07	1
Fagron	Betamethasone valerate	15I16-B07-317416	1
Fagron	Betamethasone valerate	15I16B07317417	1
Fagron	Betamethasone valerate	15I16-B07-317417	1
Fagron	Betamethasone valerate	15I16-B07-319228	2
Fagron	Betamethasone valerate	15I16-B07-319832	3
Fagron	Betamethasone valerate	15I16-Bo7-319832	1
Fagron	Betamethasone valerate	15l16-B07-319832	2
Fagron	Betamethasone valerate	16270511	1
Fagron	Betamethasone valerate	16270513	1
Fagron	Betamethasone valerate	16818-B02-320971	1
Fagron	Betamethasone valerate	16818-B02-323033	1
Fagron	Betamethasone valerate	16B18_B02-322111	1
Fagron	Betamethasone valerate	16B18-B02	6
Fagron	Betamethasone valerate	16B18-B02-320606	1
Fagron	Betamethasone valerate	16B18B02320971	1
Fagron	Betamethasone valerate	16B18-B02320971	2
Fagron	Betamethasone valerate	16B18-B02-320971	6
Fagron	Betamethasone valerate	16B18-B02-322109	5
Fagron	Betamethasone valerate	16B18-B02-322111	2
Fagron	Betamethasone valerate	16B18-B02-322121	4
Fagron	Betamethasone valerate	16B18-B02-323033	1
Fagron	Betamethasone valerate	16b18-b02-323034	1
Fagron	Betamethasone valerate	16B18-B02-323034	4
Fagron	Betamethasone valerate	16b18-b02-324798	1
Fagron	Betamethasone valerate	16B18-B02-324798	3
Fagron	Betamethasone valerate	16E23-B03	8
Fagron	Betamethasone valerate	16E23-B03-324799	8
Fagron	Betamethasone valerate	16E23-B03-3247990855	1
Fagron	Betamethasone valerate	16e23b03324800	1
Fagron	Betamethasone valerate	16e23-b03-324800	1
Fagron	Betamethasone valerate	16E23-B03-324800	12
Fagron	Betamethasone valerate	16E23-B03-327350	5
Fagron	Betamethasone valerate	16E23-B03-327354	3
Fagron	Betamethasone valerate	16E23-b03-328128	1
Fagron	Betamethasone valerate	16E23B03328128	1
Fagron	Betamethasone valerate	16E23-B03-328128	10
Fagron	Betamethasone valerate	16E23-B03-328129	2
Fagron	Betamethasone valerate	16H22-B06	3
Fagron	Betamethasone valerate	16H22-B06-329223	6
Fagron	Betamethasone valerate	16H22-B06-329231	5
Fagron	Betamethasone valerate	16H22-B06-330522	2
Fagron	Betamethasone valerate	16h22-b06-330523	2
Fagron	Betamethasone valerate	16H22-B06-330523	4
Fagron	Betamethasone valerate	16H22B06330524	2
Fagron	Betamethasone valerate	16H22-B06-330524	6
Fagron	Betamethasone valerate	16h22b06330584	1
Fagron	Betamethasone valerate	16h22-b06-331273	1
Fagron	Betamethasone valerate	16H22-B06-331273	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Betamethasone valerate	16H22-B06-332351	11
Fagron	Betamethasone valerate	16H22-B06-3332351	1
Fagron	Betamethasone valerate	170401901	1
Fagron	Betamethasone valerate	1704019-01	5
Fagron	Betamethasone valerate	17078701	1
Fagron	Betamethasone valerate	17271604	2
Fagron	Betamethasone valerate	17329001	1
Fagron	Betamethasone valerate	17329008	1
Fagron	Betamethasone valerate	17329016	1
Fagron	Betamethasone valerate	17B14-B04	1
Fagron	Betamethasone valerate	17C29-335654	1
Fagron	Betamethasone valerate	17C29-B04	7
Fagron	Betamethasone valerate	17C29-B04_336434	1
Fagron	Betamethasone valerate	17C29-B04-33368	1
Fagron	Betamethasone valerate	17C29-B04-333688	1
Fagron	Betamethasone valerate	17C29-B04-334329	10
Fagron	Betamethasone valerate	17c29-b04-335654	1
Fagron	Betamethasone valerate	17C29-B04-335654	3
Fagron	Betamethasone valerate	17c29-b04-335657	2
Fagron	Betamethasone valerate	17C29-B04-335657	11
Fagron	Betamethasone valerate	17C29B043356575581	1
Fagron	Betamethasone valerate	17C29-B04-335658	1
Fagron	Betamethasone valerate	17C29-B04-335676	6
Fagron	Betamethasone valerate	17C29-B04-336434	6
Fagron	Betamethasone valerate	17G31-B04	5
Fagron	Betamethasone valerate	17G31-B-04	1
Fagron	Betamethasone valerate	17g31-b04-338575	2
Fagron	Betamethasone valerate	17G31B04338575	1
Fagron	Betamethasone valerate	17G31-B04-338575	11
Fagron	Betamethasone valerate	17G31-B04-339784	15
Fagron	Betamethasone valerate	17G-31-B04-339784	1
Fagron	Betamethasone valerate	17G31B04339785	1
Fagron	Betamethasone valerate	17G31-B04-339785	4
Fagron	Betamethasone valerate	17G31-B04-341303	1
Fagron	Betamethasone valerate	17g31-b04-341576	3
Fagron	Betamethasone valerate	17G31B04341576	1
Fagron	Betamethasone valerate	17G31-B04-341576	12
Fagron	Betamethasone valerate	17G-31-B04-341576	1
Fagron	Betamethasone valerate	17G31-B04-341576-201	1
Fagron	Betamethasone valerate	17G31-B04-3415765	1
Fagron	Betamethasone valerate	17G31-B04-342639	1
Fagron	Betamethasone valerate	17G31-B04-344457	1
Fagron	Betamethasone valerate	17G31-B04-344757	2
Fagron	Betamethasone valerate	17K16_B08-348042	1
Fagron	Betamethasone valerate	17k16-b08	1
Fagron	Betamethasone valerate	17K16B08	1
Fagron	Betamethasone valerate	17K16-B08	11
Fagron	Betamethasone valerate	17K16-B08-344754	3
Fagron	Betamethasone valerate	17k16-b08-345541	4
Fagron	Betamethasone valerate	17K16-B08-345541	11
Fagron	Betamethasone valerate	17K16-B08-345542	1
Fagron	Betamethasone valerate	17K16-B08-345555	5
Fagron	Betamethasone valerate	17k16-B08-347309	1
Fagron	Betamethasone valerate	17K16-B08-347309	9
Fagron	Betamethasone valerate	17K-16-B08-347309	2
Fagron	Betamethasone valerate	17k16-b08-347310	1
Fagron	Betamethasone valerate	17K16-B08-347310	4
Fagron	Betamethasone valerate	17k16-b08-347912	1
Fagron	Betamethasone valerate	17k16-B08-347912	1
Fagron	Betamethasone valerate	17K16-B08-347912	10

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Betamethasone valerate	17K16-B08-348042	14
Fagron	Betamethasone valerate	17K16-B08-348538	2
Fagron	Betamethasone valerate	17K16-B08-349755	9
Fagron	Betamethasone valerate	17K16-B08-349774	1
Fagron	Betamethasone valerate	17K16-B09-345541	1
Fagron	Betamethasone valerate	17k16-bo8-347309	1
Fagron	Betamethasone valerate	17K16-BOB-345541	1
Fagron	Betamethasone valerate	18/26-B05-356852	1
Fagron	Betamethasone valerate	18/27-B05	1
Fagron	Betamethasone valerate	18/27-B05-354880	1
Fagron	Betamethasone valerate	18/27-B05-356570	1
Fagron	Betamethasone valerate	18/27-B05-356571	4
Fagron	Betamethasone valerate	18/27-B05-356584	1
Fagron	Betamethasone valerate	18/27-b05-357770	1
Fagron	Betamethasone valerate	18/27-B05-357770	1
Fagron	Betamethasone valerate	18/27-B05-358065	4
Fagron	Betamethasone valerate	18/27-B05-360081	1
Fagron	Betamethasone valerate	18/27-BO5-356570	1
Fagron	Betamethasone valerate	1811008-01	1
Fagron	Betamethasone valerate	18127-B05-358065	1
Fagron	Betamethasone valerate	1817-B05-360082	1
Fagron	Betamethasone valerate	18199907	1
Fagron	Betamethasone valerate	18G03-03-351731	1
Fagron	Betamethasone valerate	18G03-B03	6
Fagron	Betamethasone valerate	18G03-B03_351731	1
Fagron	Betamethasone valerate	18G03-B03-351450	12
Fagron	Betamethasone valerate	18G03-B03-351451	1
Fagron	Betamethasone valerate	18G03-B03-351513	3
Fagron	Betamethasone valerate	18G03-B03-351730	2
Fagron	Betamethasone valerate	18G03-B03-351731	21
Fagron	Betamethasone valerate	18G03-B03-351731	1
Fagron	Betamethasone valerate	18G03-B03-352458	1
Fagron	Betamethasone valerate	18G03-B03-352460	7
Fagron	Betamethasone valerate	18G03-B03-353212	13
Fagron	Betamethasone valerate	18I07-B05-356584	1
Fagron	Betamethasone valerate	18I27-B05	3
Fagron	Betamethasone valerate	18I27-B05_356571	1
Fagron	Betamethasone valerate	18I27-B05-354898	1
Fagron	Betamethasone valerate	18I27-B05-356570	2
Fagron	Betamethasone valerate	18i27B05356571	1
Fagron	Betamethasone valerate	18I27-B05356571	1
Fagron	Betamethasone valerate	18I27-B05-356571	5
Fagron	Betamethasone valerate	18I27-B05-356852	1
Fagron	Betamethasone valerate	18I27-B05-357770	2
Fagron	Betamethasone valerate	18I27-b05-358065	1
Fagron	Betamethasone valerate	18I27-B05-358065	5
Fagron	Betamethasone valerate	18I27-B5-356571	1
Fagron	Betamethasone valerate	18l27-B05	1
Fagron	Betamethasone valerate	18l27-B05-356584	1
Fagron	Betamethasone valerate	18l27-B05-357770	1
Fagron	Betamethasone valerate	19/26-F02-364980	1
Fagron	Betamethasone valerate	19/26-F02-364981	2
Fagron	Betamethasone valerate	19126-F02-364980	1
Fagron	Betamethasone valerate	19G03-B02-363670	1
Fagron	Betamethasone valerate	19G30-B02	17
Fagron	Betamethasone valerate	19G30B02363672	1
Fagron	Betamethasone valerate	19G30-B02-363672	8
Fagron	Betamethasone valerate	19g30-b02-363673	1
Fagron	Betamethasone valerate	19G30-B02-363673	5
Fagron	Betamethasone valerate	19G30-B02-363681	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Betamethasone valerate	19g30-b02-363682	1
Fagron	Betamethasone valerate	19G30-B02-363682	17
Fagron	Betamethasone valerate	19G30-B02-363686	5
Fagron	Betamethasone valerate	19G30-B02-363692	8
Fagron	Betamethasone valerate	19G30-B02-363693	15
Fagron	Betamethasone valerate	19G30-B03-363692	1
Fagron	Betamethasone valerate	19G30-Bo2-363693	1
Fagron	Betamethasone valerate	19GB0-B02-363693	1
Fagron	Betamethasone valerate	19I26-F02	4
Fagron	Betamethasone valerate	19I26F02364980	1
Fagron	Betamethasone valerate	19I26-F02-364980	4
Fagron	Betamethasone valerate	19I26-F02-364981	6
Fagron	Betamethasone valerate	19I26-F02-364982	1
Fagron	Betamethasone valerate	19I26-F02-364987	6
Fagron	Betamethasone valerate	19I86-F02-364987	1
Fagron	Betamethasone valerate	19J26-F02-364987	1
Fagron	Betamethasone valerate	19K11-07-366784	1
Fagron	Betamethasone valerate	19K11-F07	7
Fagron	Betamethasone valerate	19K11-F07-366779	3
Fagron	Betamethasone valerate	19k11-f07-366780	1
Fagron	Betamethasone valerate	19K11-F07-366780	1
Fagron	Betamethasone valerate	19K11-F07-3667807	1
Fagron	Betamethasone valerate	19K11-F07-3667809	1
Fagron	Betamethasone valerate	19K11-F07-366782	1
Fagron	Betamethasone valerate	19K11-F07-366784	1
Fagron	Betamethasone valerate	19k11-F07-366785	1
Fagron	Betamethasone valerate	19K11-F07-366785	16
Fagron	Betamethasone valerate	19k11f07366786	1
Fagron	Betamethasone valerate	19K11-F07-366786	9
Fagron	Betamethasone valerate	19K11-F07-366787	5
Fagron	Betamethasone valerate	19K11-F07-366788	3
Fagron	Betamethasone valerate	19K11-F07-366788	1
Fagron	Betamethasone valerate	19K11-F07-366789	3
Fagron	Betamethasone valerate	19K11-Fo7-366785	1
Fagron	Betamethasone valerate	19K11-FO7-366785	1
Fagron	Betamethasone valerate	19K-F0-366786	1
Fagron	Betamethasone valerate	19l26-F02	3
Fagron	Betamethasone valerate	19l26-F02-364981	1
Fagron	Betamethasone valerate	19l26-F02-364986	1
Fagron	Betamethasone valerate	19UI26-F02-364981	1
Fagron	Betamethasone valerate	2000036016	1
Fagron	Betamethasone valerate	20101012-1	1
Fagron	Betamethasone valerate	20818-F07	1
Fagron	Betamethasone valerate	20B18-F07	5
Fagron	Betamethasone valerate	20B18-F07-3696704	2
Fagron	Betamethasone valerate	20B18-F07-369671	2
Fagron	Betamethasone valerate	20B18-F07-369673	17
Fagron	Betamethasone valerate	20B18-F07-369674	1
Fagron	Betamethasone valerate	20B18-F07-369676	3
Fagron	Betamethasone valerate	20B18-F07-3700009	1
Fagron	Betamethasone valerate	20B18-F07-370009	6
Fagron	Betamethasone valerate	20B18-F07-370010	2
Fagron	Betamethasone valerate	20B18F07370013	1
Fagron	Betamethasone valerate	20B18-F07-370013	3
Fagron	Betamethasone valerate	20B18-F07-37009	1
Fagron	Betamethasone valerate	20E14-F02	3
Fagron	Betamethasone valerate	20E14-F02-371690	13
Fagron	Betamethasone valerate	20E14-F02-372350	7
Fagron	Betamethasone valerate	20G17-F02	3
Fagron	Betamethasone valerate	20G17-F02-3737909	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Betamethasone valerate	20G17-F02-373798	7
Fagron	Betamethasone valerate	20G17-F02-373799	5
Fagron	Betamethasone valerate	21000036020	1
Fagron	Betamethasone valerate	2152-44-5	1
Fagron	Betamethasone valerate	21D09-F03	3
Fagron	Betamethasone valerate	21D09-F03-377824	7
Fagron	Betamethasone valerate	21D09-F03-377825	4
Fagron	Betamethasone valerate	21D09-F03377843	1
Fagron	Betamethasone valerate	21D09-F03-377843	1
Fagron	Betamethasone valerate	21G28-B02	1
Fagron	Betamethasone valerate	21G28-B02-213513	1
Fagron	Betamethasone valerate	21G28-B02-213516	9
Fagron	Betamethasone valerate	21G28-B02-213517	4
Fagron	Betamethasone valerate	21G28-B02-213518	6
Fagron	Betamethasone valerate	21G28-B02-213663	2
Fagron	Betamethasone valerate	21G28-BO2-213518	1
Fagron	Betamethasone valerate	21K09_B05_218135	1
Fagron	Betamethasone valerate	21K09B05	1
Fagron	Betamethasone valerate	21K09-B05	1
Fagron	Betamethasone valerate	21K09-B05-217883	8
Fagron	Betamethasone valerate	21K09B05217891	1
Fagron	Betamethasone valerate	21K09-B05-217891	8
Fagron	Betamethasone valerate	21K09-B05-217898	2
Fagron	Betamethasone valerate	21K09-B05-218135	1
Fagron	Betamethasone valerate	21K09-B05-220180	7
Fagron	Betamethasone valerate	21K09B05220215	1
Fagron	Betamethasone valerate	21K09-B05-220215	5
Fagron	Betamethasone valerate	21K09-B05-220334	1
Fagron	Betamethasone valerate	21K09-B05-220365	2
Fagron	Betamethasone valerate	21K09-B05-2221193	1
Fagron	Betamethasone valerate	21K09-B05-222192	4
Fagron	Betamethasone valerate	21K09-B05-222194	1
Fagron	Betamethasone valerate	22H25B07	1
Fagron	Betamethasone valerate	22H25-B07	1
Fagron	Betamethasone valerate	22H25B07223527	4
Fagron	Betamethasone valerate	22H25-B07-223527	4
Fagron	Betamethasone valerate	22H25-B07-223537	1
Fagron	Betamethasone valerate	22H25B072235527	1
Fagron	Betamethasone valerate	292652	1
Fagron	Betamethasone valerate	2B28-N01	1
Fagron	Betamethasone valerate	2OB18-F07-370009	1
Fagron	Betamethasone valerate	309520	1
Fagron	Betamethasone valerate	364979	1
Fagron	Betamethasone valerate	612211181	1
Fagron	Betamethasone valerate	700103-0002	3
Fagron	Betamethasone valerate	700103-0003	1
Fagron	Betamethasone valerate	700103-0004	2
Fagron	Betamethasone valerate	90616-2	1
Fagron	Betamethasone valerate	B02-3636307	1
Fagron	Betamethasone valerate	b02-3636702	1
Fagron	Betamethasone valerate	B02-3636802	1
Fagron	Betamethasone valerate	B05-217898	1
Fagron	Betamethasone valerate	B05-2203305	1
Fagron	Betamethasone valerate	B07-317416	1
Fagron	Betamethasone valerate	BO5-2203305	1
Fagron	Betamethasone valerate	BV004/0721	2
Fagron	Betamethasone valerate	BV008/0415	1
Fagron	Betamethasone valerate	BV008/045	1
Fagron	Betamethasone valerate	BV008/0516	1
Fagron	Betamethasone valerate	BV009/0117	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Betamethasone valerate	BV019/0514	3
Fagron	Betamethasone valerate	BV036/1215	1
Fagron	Betamethasone valerate	BV102/0420	6
Fagron	Betamethasone valerate	BV106/0717	2
Fagron	Betamethasone valerate	BV109/0117	2
Fagron	Betamethasone valerate	BV109/0519	6
Fagron	Betamethasone valerate	BV110/0818	1
Fagron	Betamethasone valerate	BV123/0120	2
Fagron	Betamethasone valerate	BV124/0118	2
Fagron	Betamethasone valerate	BV127/0120	1
Fagron	Betamethasone valerate	BV-BLT225/0514	1
Fagron	Betamethasone valerate	BV-BLT250/0616	2
Fagron	Betamethasone valerate	F02-3649807	2
Fagron	Betamethasone valerate	F02-3716900	1
Fagron	Betamethasone valerate	F02-3723500	1
Fagron	Betamethasone valerate	F02-3737908	1
Fagron	Betamethasone valerate	F02-3737909	2
Fagron	Betamethasone valerate	F03377824	1
Fagron	Betamethasone valerate	F07-3667805	1
Fagron	Betamethasone valerate	F07-3667808	1
Fagron	Betamethasone valerate	F07-3696703	1
Fagron	Betamethasone valerate	F07-3700100	1
Fagron	Betamethasone valerate	F073700103	1
Fagron	Betamethasone valerate	fagron	1
Fagron	Betamethasone valerate	NP1351M	1
Fagron	Betamethasone valerate	NS0706M	3
Fagron	Betamethasone valerate	NS2072M	1
Fagron	Betamethasone valerate	NT0597M	4
Fagron	Betamethasone valerate	NT059M	1
Fagron	Betamethasone valerate	Op07062022B	1
Fargon, Noweda 07.11.2017	Betamethasone valerate	16H22-B06-329223	1
Fargon/AHD	Betamethasone valerate	18/27-B05	1
Fargon/Alliance HC	Betamethasone valerate	13K29-B32-288247	1
Fargon/Alliance HC	Betamethasone valerate	16B18-B02-322111	1
Fargon/Anzag	Betamethasone valerate	13G19-N01	1
Fargon/Anzag	Betamethasone valerate	16B18-B02-320971	1
Fargon/Noweda	Betamethasone valerate	18I27-B05-354898	1
Fargon	Betamethasone valerate	13k29-b32-289364	1
Fargon	Betamethasone valerate	18g03-b03-351731	1
Fargon	Betamethasone valerate	19G30-B08-36393	1
Fargon	Betamethasone valerate	20G17-F02-373798	1
Fargon	Betamethasone valerate	21K09-B05-217883	1
Fargon	Betamethasone valerate	7890	1
Fargron	Betamethasone valerate	13G19-N01	1
Fargron	Betamethasone valerate	13K29-B32-288246	1
Farmabios S. p. A./ ...	Betamethasone valerate	17078715	1
Farmabios S.p.A., IT	Betamethasone valerate	2109VM00012222	1
Farmabios spa	Betamethasone valerate	19220704	1
Farmabios/Noweda	Betamethasone valerate	2109VM0B0011722	1
Farmabios/Noweda	Betamethasone valerate	2109VMOB0011722	1
Farmabios/Phoenix	Betamethasone valerate	2109VMOCO011922	1
Farmabios	Betamethasone valerate	17271603	1
Fiebig 27.06.13 EK47,81	Betamethasone valerate	B9/131	1
Fiebig ek: 45,65EUR	Betamethasone valerate	12B28-N01	1
Fiebig/Farago	Betamethasone valerate	19G30-B02-363692	1
Fiebig	Betamethasone valerate	14H28-B01	1
Fiebig	Betamethasone valerate	15B24-B04-307016	1
Fiebig	Betamethasone valerate	16B18-B02-322111	1
Fiebig	Betamethasone valerate	17271603	1
FIEBIG	Betamethasone valerate	F17-3696703	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Finteler Apotheke	Betamethasone valerate	17C29-B04-333688	2
Fragon/ Gehe	Betamethasone valerate	19K11-F07-366785	1
Fragon/Alliance	Betamethasone valerate	17k16-B08	1
Fragon/Phönix	Betamethasone valerate	17G31-B04-341576	1
Fragon/Sanacorp	Betamethasone valerate	17K16-B08-340842	1
Fragon	Betamethasone valerate	16G03-B03-353212	1
Fragon	Betamethasone valerate	19K11-F07-366784	1
Fragron	Betamethasone valerate	BV-BLT225/0514	2
Galderma/ Noweda	Betamethasone valerate	C0023/115040	1
Gatt-Koller	Betamethasone valerate	1800117	1
GEHE 17.06.2014	Betamethasone valerate	13225503	1
Gehe am 03.02.2014	Betamethasone valerate	13091210	3
Gehe amax	Betamethasone valerate	18199930	1
Gehe	Betamethasone valerate	12003403	1
Gehe	Betamethasone valerate	12003409	1
Gehe	Betamethasone valerate	1208014-04	1
Gehe	Betamethasone valerate	12229809	1
Gehe	Betamethasone valerate	13091211	1
Gehe	Betamethasone valerate	14H25-B01-302863	1
Gehe	Betamethasone valerate	14H28-B01-302863	1
Gehe	Betamethasone valerate	15075804	1
Gehe	Betamethasone valerate	15075811	1
Gehe	Betamethasone valerate	15398501	1
Gehe	Betamethasone valerate	15398512	1
GEHE	Betamethasone valerate	16270501	1
Gehe	Betamethasone valerate	16270505	1
Gehe	Betamethasone valerate	16H22-B06	1
Gehe	Betamethasone valerate	16H22-B06-330524	1
GEHE	Betamethasone valerate	17078701	2
Gehe	Betamethasone valerate	17078703	1
Gehe	Betamethasone valerate	17078712	1
GEHE	Betamethasone valerate	17078719	1
GEHE	Betamethasone valerate	17078720	1
Gehe	Betamethasone valerate	1712E-01181	1
Gehe	Betamethasone valerate	17271603	1
Gehe	Betamethasone valerate	17329015	1
Gehe	Betamethasone valerate	17329018	1
Gehe	Betamethasone valerate	17G31-B04	1
Gehe	Betamethasone valerate	17K16-B08	1
Gehe	Betamethasone valerate	17K16-B08-347309	1
Gehe	Betamethasone valerate	17K16-B08-348042	1
Gehe	Betamethasone valerate	1811008-01	1
GEHE	Betamethasone valerate	18199902	2
Gehe	Betamethasone valerate	18199908	1
Gehe	Betamethasone valerate	18199924	3
gehe	Betamethasone valerate	18199937	1
Gehe	Betamethasone valerate	18G03-B03-351731	1
Gehe	Betamethasone valerate	18I27-B05	1
Gehe	Betamethasone valerate	192207001	2
Gehe	Betamethasone valerate	192207002	1
Gehe	Betamethasone valerate	19220702	1
Gehe	Betamethasone valerate	21K09-b05	1
gehe	Betamethasone valerate	21K09-B05-220180	1
Gehe	Betamethasone valerate	21K09-B05-22192	1
GEHE	Betamethasone valerate	22001101015	1
Gehe	Betamethasone valerate	22001101016	1
Gehe	Betamethasone valerate	22001101021	1
Gehe	Betamethasone valerate	2202016-01	2
Gehe	Betamethasone valerate	2202016-02	1
gehe	Betamethasone valerate	22H25B07227237	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Betamethasone valerate	22K07-B08-229283	1
Gehe	Betamethasone valerate	22K07-B08-233606	1
Gehe	Betamethasone valerate	2309023-01	1
Gehe	Betamethasone valerate	23E29-B03-235955	1
Gehe	Betamethasone valerate	23E29-B03-238320	1
Gehe	Betamethasone valerate	BV001/0322	1
Geilenkirchen	Betamethasone valerate	16270513	1
Geilenkirchen	Betamethasone valerate	17078701	1
Geilenkirchen	Betamethasone valerate	18199918	1
Hedinger / Noweda	Betamethasone valerate	16270505	1
Hedinger	Betamethasone valerate	14H28-B01-302877	1
Hepart AG, CH-8280 K...	Betamethasone valerate	11131914	3
Hirsch	Betamethasone valerate	13G19-No1	1
Holdermann	Betamethasone valerate	1208014-01	1
Holdermann	Betamethasone valerate	120801402	1
Ichthyol-Gesellschaft	Betamethasone valerate	13k29-B32-288247	1
Ichthyol-Gesellschaft	Betamethasone valerate	17078720	1
jenne/eurho	Betamethasone valerate	2102010-01	1
Jenne	Betamethasone valerate	17078712	1
Jenne	Betamethasone valerate	1811008-01	3
Jenne	Betamethasone valerate	18199918	1
Jenne	Betamethasone valerate	18199933	1
Jenne	Betamethasone valerate	18I27-B05-358065	1
Jenne	Betamethasone valerate	21000036017	1
Jenne	Betamethasone valerate	22001101004	1
Jenne	Betamethasone valerate	22001101020	1
Kehr	Betamethasone valerate	1801024-01	1
Kehr	Betamethasone valerate	22001101015	1
Kehr	Betamethasone valerate	22001101020	1
Kehr	Betamethasone valerate	2202016-01	1
Kehr	Betamethasone valerate	22H25-07-227224	1
Klenk	Betamethasone valerate	16623-01	1
Klenk	Betamethasone valerate	17078713	1
Klenk	Betamethasone valerate	17078714	1
Klosterring	Betamethasone valerate	18199916	2
Krieger	Betamethasone valerate	192207010	1
krieger	Betamethasone valerate	20G17-F02-373798	1
L12	Betamethasone valerate	16E23-B03-324799	2
L12	Betamethasone valerate	17C29-B04-334329	2
L12	Betamethasone valerate	17K16-B08-345541	1
Lamotte/Noweda	Betamethasone valerate	17K16-B08-349755	1
Midas	Betamethasone valerate	16270503	1
Midas	Betamethasone valerate	16270513	1
Midas	Betamethasone valerate	17078712	2
Midas	Betamethasone valerate	17078720	1
Midas	Betamethasone valerate	17329001	2
Midas	Betamethasone valerate	17329018	1
Midas	Betamethasone valerate	17G31-B04-338575	2
Mömerzheim	Betamethasone valerate	17329008	1
NEWCHEM	Betamethasone valerate	1311039-01	1
Noveda	Betamethasone valerate	1311039-01	1
Noveda	Betamethasone valerate	192207002	1
Noweda/ Infecto Pharm	Betamethasone valerate	16270505	1
Noweda/cealo	Betamethasone valerate	17329002	1
Noweda/Ceasar Lorenz	Betamethasone valerate	14188606	1
Noweda	Betamethasone valerate	11131902	1
Noweda	Betamethasone valerate	11B21-N02	1
Noweda	Betamethasone valerate	1208014-01	1
Noweda	Betamethasone valerate	1208014-02	2
noweda	Betamethasone valerate	1208014-04	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Betamethasone valerate	12229832	1
Noweda	Betamethasone valerate	12G09-N07	1
Noweda	Betamethasone valerate	13091203	1
Noweda	Betamethasone valerate	13091205	1
noweda	Betamethasone valerate	1406019-01	1
Noweda	Betamethasone valerate	1406019-03	2
Noweda	Betamethasone valerate	14H28B01302863	1
Noweda	Betamethasone valerate	15075812	1
Noweda	Betamethasone valerate	161001001	1
Noweda	Betamethasone valerate	16270511	1
Noweda	Betamethasone valerate	1704019-01	1
Noweda	Betamethasone valerate	17078701	1
Noweda	Betamethasone valerate	17271601	2
Noweda	Betamethasone valerate	17329018	2
Noweda	Betamethasone valerate	17g31-b04-338575	1
Noweda	Betamethasone valerate	1801024-01	2
Noweda	Betamethasone valerate	1811008-01	2
Noweda	Betamethasone valerate	18199918	1
Noweda	Betamethasone valerate	18199932	3
Noweda	Betamethasone valerate	18199933	1
Noweda	Betamethasone valerate	18127-B05-354880	1
Noweda	Betamethasone valerate	1912012-01	1
Noweda	Betamethasone valerate	19220704	2
Noweda	Betamethasone valerate	19220705	2
Noweda	Betamethasone valerate	19I26-F02-364981	1
Noweda	Betamethasone valerate	20G17-F02-373798	1
Noweda	Betamethasone valerate	21000036003	1
Noweda	Betamethasone valerate	21K09-B05	1
Noweda	Betamethasone valerate	22001101003	1
Noweda	Betamethasone valerate	2202016-01	6
Noweda	Betamethasone valerate	22K07-08-229283	1
Noweda	Betamethasone valerate	2309023	1
Noweda	Betamethasone valerate	2309023-01	2
Noweda	Betamethasone valerate	BV01090117	1
Oberlinden- Apotheke	Betamethasone valerate	C0073/1	3
Oberlinden Apotheke	Betamethasone valerate	C0073/115040	3
Oberlinden Apotheke	Betamethasone valerate	c073/115040	1
Phoenix 15.1.2014	Betamethasone valerate	1208014-04	1
Phoenix 13.12.2017	Betamethasone valerate	16H22-B06-330524	1
Phoenix 22.01.2019	Betamethasone valerate	1801021-01	1
Phoenix 30.10.19 19,34EUR	Betamethasone valerate	18/27-B05-358065	1
Phoenix Goettin	Betamethasone valerate	13225508	1
Phoenix/ Fagro	Betamethasone valerate	18G03-B03-351731	1
Phoenix	Betamethasone valerate	12003409	2
Phoenix	Betamethasone valerate	16270513	1
Phoenix	Betamethasone valerate	170401901	1
Phoenix	Betamethasone valerate	17329002	1
Phoenix	Betamethasone valerate	17329018	1
Phoenix	Betamethasone valerate	17C29-B04-334329	1
Phoenix	Betamethasone valerate	17K16-B08-348042	2
Phoenix	Betamethasone valerate	1801024-01	1
Phoenix	Betamethasone valerate	1811008-01	2
Phoenix	Betamethasone valerate	18127-B05-358065	1
Phoenix	Betamethasone valerate	191201201	1
Phoenix	Betamethasone valerate	192207003	1
Phoenix	Betamethasone valerate	192207009	1
Phoenix	Betamethasone valerate	19220705	1
Phoenix	Betamethasone valerate	19G30-B02-363672	2
Phoenix	Betamethasone valerate	19G30-B02-363682	1
Phoenix	Betamethasone valerate	19K11-F07	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Betamethasone valerate	19126-F02-3649800	1
Phoenix	Betamethasone valerate	200592406	1
Phoenix	Betamethasone valerate	2102010-01	1
Phoenix	Betamethasone valerate	22001101016	2
Phoenix	Betamethasone valerate	3105	1
Phoenix	Betamethasone valerate	3364	1
Phönix Gotha	Betamethasone valerate	12229808	1
Phönix Gotha	Betamethasone valerate	13091213	1
Phönix Gotha	Betamethasone valerate	14188608	1
Phönix Gotha	Betamethasone valerate	1704019-01	1
Phönix Gotha	Betamethasone valerate	1811008-01	1
Phönix WE:16.07.2016...	Betamethasone valerate	1510037-01	1
Phönix	Betamethasone valerate	12229807	1
Phönix	Betamethasone valerate	13091201	2
Phönix	Betamethasone valerate	13091209	2
Phönix	Betamethasone valerate	13091212	2
Phönix	Betamethasone valerate	13D03-N07	1
Phonix	Betamethasone valerate	13K29-B32	1
phönix	Betamethasone valerate	15/16B07-319228	1
Phönix	Betamethasone valerate	15075804	1
Phönix	Betamethasone valerate	1507804	1
phönix	Betamethasone valerate	15398515	1
Phönix	Betamethasone valerate	16270503	1
phönix	Betamethasone valerate	16e23-b03-327350	1
Phönix	Betamethasone valerate	16H22-B06-330522	1
Phönix	Betamethasone valerate	17078712	1
Phönix	Betamethasone valerate	17329001	1
Phönix	Betamethasone valerate	18199907	1
Phönix	Betamethasone valerate	18199918	1
Phönix	Betamethasone valerate	18199933	1
Phönix	Betamethasone valerate	1911001-01	2
Phönix	Betamethasone valerate	192207009	1
Phönix	Betamethasone valerate	19220705	1
Phönix	Betamethasone valerate	19g30-b02-363672	1
Phönix	Betamethasone valerate	19G30-B02-363693	1
Phönix	Betamethasone valerate	19I26-F02-0364979	2
Phönix	Betamethasone valerate	19I26-F02-364981	1
Phönix	Betamethasone valerate	19K11-F07-366779	1
PHÖNIX	Betamethasone valerate	19K11-F07-366785	1
Phönix	Betamethasone valerate	19K11-F07-366786	1
Phönix	Betamethasone valerate	19K11-F07-366787	2
Phönix	Betamethasone valerate	19K11-F07-366789	1
Phönix	Betamethasone valerate	20E14-F02-371690	1
Phönix	Betamethasone valerate	21K09-B05-220215	1
Phönix	Betamethasone valerate	22001101009	1
Phönix	Betamethasone valerate	22001101018	1
Phönix	Betamethasone valerate	22001101020	2
Phönix	Betamethasone valerate	22001101021	1
Phönix	Betamethasone valerate	2202016-02	1
Phönix	Betamethasone valerate	B02-3636802	1
Phönix	Betamethasone valerate	BV110/0818	1
Phönix	Betamethasone valerate	BV-BLT186/0512	1
Phönix	Betamethasone valerate	F07-3696701	1
Röntgen	Betamethasone valerate	1911001-01	4
Sanacorp W.E: 18.01....	Betamethasone valerate	1704019-01	1
Sanacorp	Betamethasone valerate		1
Sanacorp	Betamethasone valerate	12G09-N07	1
Sanacorp	Betamethasone valerate	13091210	1
Sanacorp	Betamethasone valerate	13225503	1
Sanacorp	Betamethasone valerate	14188602	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Betamethasone valerate	14G30-B05-296173	1
Sanacorp	Betamethasone valerate	16H22-B06-330522	1
Sanacorp	Betamethasone valerate	1704019-01	1
Sanacorp	Betamethasone valerate	17078715	1
Sanacorp	Betamethasone valerate	17078719	1
Sanacorp	Betamethasone valerate	17C29-B04	1
Sanacorp	Betamethasone valerate	1801024-01	4
Sanacorp	Betamethasone valerate	1811008	2
Sanacorp	Betamethasone valerate	1811008-01	7
Sanacorp	Betamethasone valerate	18199918	2
Sanacorp	Betamethasone valerate	18199933	3
Sanacorp	Betamethasone valerate	192207010	1
Sanacorp	Betamethasone valerate	19220705	1
Sanacorp	Betamethasone valerate	19G30-B02-3636706	1
Sanacorp	Betamethasone valerate	19G30-B02-3636806	1
Sanacorp	Betamethasone valerate	19I26f02364981	1
Sanacorp	Betamethasone valerate	21000036017	1
Sanacorp	Betamethasone valerate	2100036021	1
Sanacorp	Betamethasone valerate	2102010-02	1
Sanacorp	Betamethasone valerate	22K07-B08-233606	1
Sanacorp	Betamethasone valerate	30051201	1
Sanacorp	Betamethasone valerate	F07-3700100	1
Spangro 31.05.2013	Betamethasone valerate	13D03-N07	2
Spangro	Betamethasone valerate	17078714	1
Spangro_21.05.2019	Betamethasone valerate	1811008-01	3
Symbiotica / Gehe	Betamethasone valerate	BV018/0715	1
Symbiotica / Gehe	Betamethasone valerate	BV036/1215	1
Symbiotica / Sanacorp	Betamethasone valerate	18I27-B05-354898	2
Symbiotica Spec.	Betamethasone valerate	1208014-04	1
Symbiotica Spec.	Betamethasone valerate	1406019-01	3
Symbiotica/ Anzag	Betamethasone valerate	1606023-01	2
Symbiotica/ Phönix	Betamethasone valerate	2102010-01	3
Symbiotica/Gehe	Betamethasone valerate	1912012-01	1
Symbiotica	Betamethasone valerate	14H28B01302863	1
Symbiotica	Betamethasone valerate	1610010-01	2
Symbotica Spec/Noweda	Betamethasone valerate	1208014-04	1
vdl	Betamethasone valerate	12003411	1

- 230 446 spectra from 1515 *Apo-Ident* customers from a total of 48 411 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Betamethasone valerate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Betamethasone valerate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	554	0	152 408
Type B	0	881	0	201 203
Type C	0	5546	75	230 446

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The substance/substance group *Betamethasone valerate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9170 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.3190 %)
Type C	100.0000 % (> 99.9007 %)	98.6657 % (> 98.6123 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20887	22249	8.97	103.83
20920	22249	10.19	115.83
21215	22249	8.68	115.14
21566	22249	7.71	113.56
21588	21588	0.00	109.14
21645	22249	6.83	110.85
21674	21674	0.00	142.65
22249	22249	0.00	111.36
22861	22861	0.00	114.47
24349	24349	0.00	106.58

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Bifonazole**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20810-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bifonazole; Bifonazolum

Special notes

When selecting the *Bifonazole* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Bifonazole	8	5	75

Second-stage model

For differentiation of the substance/substance group *Bifonazole* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Bifonazole* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Clotrimazole	30.04	–
Methoxsalen	145.52	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Bifonazole* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Bifonazole*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Bifonazole	15152701	22906	40	20150703
Caelo	Bifonazole	15152702	22907	40	20150703
Caelo	Bifonazole	15152702	22955	40	20150703
Caelo	Bifonazole	151527	23364	40	20150703*
Euro OTC	Bifonazole	1206027-01	20810	40	1312397
Euro OTC	Bifonazole	1401031-01	21631	60	20140220
Euro OTC	Bifonazole	1510001	22253	60	20151203*
Fagron	Bifonazole	12G11-N09	20820	40	20120807
Fagron	Bifonazole	16D07-B10-324381	22941	40	20160419

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 400 spectra of 9 reference samples from the substance/substance group *Bifonazole*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 562 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Bifonazole*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Bifonazole	182771	24365	40
Caelo	Bifonazole	22001498	26738	40
Euro OTC	Bifonazole	1703041	23395	40
Euro OTC	Bifonazole	1806008	24161	40
Fagron	Bifonazole	22C23-B03-219763	26376	40
Caelo	Bifonazole	22001498	26738SI	20
Fagron	Bifonazole	22C23-B03-219763	26376SI	20

- 201 844 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 211 spectra from 81 *Apo-Ident* customers from 84 batches from the substance/substance group *Bifonazole*.

- Among them are spectra of independent samples from 75 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Bifonazole	21B18-B03-228686	2
	Bifonazole	22001498010	1
	Bifonazole	22C23-B03-223797	2
	Bifonazole	22L06-B10-223798	2
Caelo	Bifonazole	13I09-N07	1
Caelo	Bifonazole	14k10-B01-312067	1
Caelo	Bifonazole	15152701	6
Caelo	Bifonazole	16J03-B08-331029	1
Caelo	Bifonazole	1703041-01	2
Caelo	Bifonazole	18009702	9
Caelo	Bifonazole	18009704	4
Caelo	Bifonazole	18009705	1
Caelo	Bifonazole	18277103	1
Caelo	Bifonazole	18277104	1
Caelo	Bifonazole	19287504	1
Caelo	Bifonazole	19287505	2
Caelo	Bifonazole	20003802002	3
Caesar & Loretz GmbH...	Bifonazole	18277104	1
Caesar & Loretz GmbH...	Bifonazole	19287505	1
Caesar & Loretz GmbH	Bifonazole	18277104	1
Caesar & Loretz GmbH	Bifonazole	19287505	2
Caesar & Loretz GmbH	Bifonazole	20003802002	2
Erregierre S.p.A	Bifonazole	A200003	2
Euro OTC	Bifonazole	1206027-01	2
Euro OTC	Bifonazole	1206027-02	1
Euro OTC	Bifonazole	13G10N02	1
Euro OTC	Bifonazole	1510001-02	6
Euro OTC	Bifonazole	16703-B08-333937	1
Euro OTC	Bifonazole	170304101	1
Euro OTC	Bifonazole	1703041-01	5
Euro OTC	Bifonazole	18041814	1
Euro OTC	Bifonazole	1806008-01	12
Euro OTC	Bifonazole	18065008-01	1
Euro Rho/Jenne	Bifonazole	1806008-011	1
Fagron	Bifonazole		2
Fagron	Bifonazole	11F20-N06	1
Fagron	Bifonazole	12D17-N02	3
Fagron	Bifonazole	12E29-N03	5
Fagron	Bifonazole	12G11-N09	2
Fagron	Bifonazole	13G10-N02	2
Fagron	Bifonazole	14C28-B03-292388	1
Fagron	Bifonazole	14C28-B03-292389	1
Fagron	Bifonazole	14K10-B01-300541	6
Fagron	Bifonazole	14K10-B01-306783	5
Fagron	Bifonazole	14K10-B01-308349	2
Fagron	Bifonazole	14K10-B01-312067	2
Fagron	Bifonazole	14K10-B01-316618	1
Fagron	Bifonazole	15/18-B04-320085	1
Fagron	Bifonazole	1518-B04-316619	1
Fagron	Bifonazole	15I18-B04-316619	1
Fagron	Bifonazole	1607-B10-324380	1
Fagron	Bifonazole	16D07-B10-321576	2
Fagron	Bifonazole	16D07-B10-324380	3
Fagron	Bifonazole	16D07-B10-324381	6
Fagron	Bifonazole	16D07-B10-32480	1
Fagron	Bifonazole	16j03-b08-327046	2
Fagron	Bifonazole	16J03-B08-327046	4
Fagron	Bifonazole	16J03-B08-331029	2
Fagron	Bifonazole	16J03-B08-333936	2
Fagron	Bifonazole	16J03-B08-333937	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Bifonazole	18A15-B05	1
Fagron	Bifonazole	18A15-B05_344514	1
Fagron	Bifonazole	18A15-B05-344515	4
Fagron	Bifonazole	18A15-B05-347176	2
Fagron	Bifonazole	18A15-B05-350644	1
Fagron	Bifonazole	18A15-B05-353060	2
Fagron	Bifonazole	18A15-B05-357230	1
Fagron	Bifonazole	18A15-B05-357781	2
Fagron	Bifonazole	18A15-B05-358736	2
Fagron	Bifonazole	18A15-B05-362358	1
Fagron	Bifonazole	18A15-B5-34716	1
Fagron	Bifonazole	19E06B01363093	1
Fagron	Bifonazole	19E06-B01-363093	7
Fagron	Bifonazole	19E06-B01-367109	2
Fagron	Bifonazole	19L04-F02-369242	8
Fagron	Bifonazole	19L-F02-369242	1
Fagron	Bifonazole	20L03-F03-375885	7
Fagron	Bifonazole	20L03-F03-375887	1
Fagron	Bifonazole	21B18-B03-215543	4
Fagron	Bifonazole	22C23-B03-223797	1
Fagron	Bifonazole	A160002	1
Fagron	Bifonazole	A170003	1
Fagron	Bifonazole	A190005	1
Fagron	Bifonazole	A200003	1
Fagron	Bifonazole	B05-3623508	1
Fagron	Bifonazole	f02-3671100	2
Fargon	Bifonazole	14k10-b01-300541	1
Gehe	Bifonazole	13D12-N11	1
Gehe	Bifonazole	15152703	1
Gehe	Bifonazole	19L04-F02-369242	1
Gehe	Bifonazole	20003802009	1
Noweda	Bifonazole	18A15-B05-344514	1
Sanacorp	Bifonazole	19287505	1
Sanacorp	Bifonazole	19E06-B01	1

- 235 856 spectra from 1515 *Apo-Ident* customers from a total of 49 174 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Bifonazole* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bifonazole* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	240	0	201 844
Type C	0	208	3	235 856

The substance/substance group *Bifonazole* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	98.5782 % (> 97.1564 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20810	20810	0.00	64.26
20820	23364	12.22	60.98
21631	20810	9.03	66.72
22253	22253	0.00	66.68
22906	22253	6.50	61.71
22907	23364	4.80	63.36
22941	23364	4.40	62.83
22955	23364	3.06	63.13
23364	23364	0.00	64.04

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Biotin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20414-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Biotin; Biotinum

Special notes

When selecting the *Biotin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Biotin	8	16	56

Second-stage model

For differentiation of the substance/substance group *Biotin* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Biotin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	124.18	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Biotin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Biotin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Biotin	16164313	22901	40	20160616
Caelo	Biotin	16164313	22902	40	20160216
Caelo	Biotin	163432	23029	40	20170119*
Caelo	Biotin	163432	23063	40	20170119*
Euro OTC	Biotin	1402028-01	21632	60	20140404
Euro OTC	Biotin	1508030	21904	60	20150925*
Euro OTC	Biotin	1610003	22855	40	20161110*
Euro OTC	Biotin	2009044	25536	40	20210215*
Fagron	Biotin	13K29-N02	21221	40	20131204
Fagron	Biotin	17K20-B03-351524	24694	40	20180108

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 440 spectra of 10 reference samples from the substance/substance group *Biotin*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

batches.

- 152 522 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 710 spectra of 19 reference samples from the substance/substance group *Biotin*.

- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Biotin	173152	23829	40
Caelo	Biotin	183009	24372	40
Caelo	Biotin	21003208	25850	50
Caelo	Biotin	24000895	27224	40
Caelo	Biotin	23003236	27228	40
Euro OTC	Biotin	1603017	22507	40
Euro OTC	Biotin	1708007	23728	40
Euro OTC	Biotin	1802022	23955	40
Euro OTC	Biotin	1903020	24612	40
Euro OTC	Biotin	1903019	24631	40
Euro OTC	Biotin	2005032	25420	40
Euro OTC	Biotin	2110003	25875	50
Euro OTC	Biotin	2306005	26934	40
Euro OTC	Biotin	2311005	27146	40
Fagron	Biotin	22C02-B01-217682	26157	40
Fagron	Biotin	24D08-B01-236877	27374	40
Euro OTC	Biotin	2110003	25875SI	10
Euro OTC	Biotin	2306005	26934SI	20
Fagron	Biotin	22C02-B01-217682	26157SI	20

- 201 374 spectra from a total of 4029 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 123 spectra from 38 *Apo-Ident* customers from 60 batches from the substance/substance group *Biotin*.

- Among them are spectra of independent samples from 56 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Biotin	2009044-03	1
	Biotin	21002482008	1
	Biotin	22C02-B01-224530	1
	Biotin	22C02-B01-217682	1
	Biotin	2306005-02	3
	Biotin	24000895001	1
Caelo	Biotin	12A23-N03	1
Caelo	Biotin	13K29-N02	2
Caelo	Biotin	1402028-01	2
Caelo	Biotin	1610003-02	1
Caelo	Biotin	1708007-01	2
Caelo	Biotin	17D28-B07-334630	1
EuRho	Biotin	1802022-01	1
Euro OTC	Biotin	10061709	1
Euro OTC	Biotin	1111039-02	1
Euro OTC	Biotin	1301026-01	3
Euro OTC	Biotin	1402028-01	2
Euro OTC	Biotin	1411047-01	3
Euro OTC	Biotin	1508030-01	2
Euro OTC	Biotin	1603017-01	1
Euro OTC	Biotin	161000301	1
Euro OTC	Biotin	1610003-01	6
Euro OTC	Biotin	170800701	1
Euro OTC	Biotin	1708007-01	8
Euro OTC	Biotin	180202201	6
Euro OTC	Biotin	1802022-01	4
Euro OTC	Biotin	1802022-02	3
Euro OTC	Biotin	1802022-03	1
Euro OTC	Biotin	1903019-01	5
Euro OTC	Biotin	190302001	1
Euro OTC	Biotin	1903020-01	4
Euro OTC	Biotin	2009044-01	14
Euro OTC	Biotin	2009044-02	1
Euro OTC	Biotin	2041517	1
Euro OTC	Biotin	2110003	1
Euro OTC	Biotin	2110003-01	7
Euro OTC	Biotin	24011801	1
Euro OTC	Biotin	2417Q-01100	1
Euro OTC	Biotin	28071506	1
Euro OTC	Biotin	2818Q-01100	1
Euro OTC	Biotin	3021501	1
Euro OTC	Biotin	5121812	1
Fagron	Biotin	12111302	1
Fagron	Biotin	12A23-N03	1
Fagron	Biotin	12C14-N01	1
Fagron	Biotin	13081203	1
Fagron	Biotin	13111202	1
Fagron	Biotin	14d04-b07-292963	1
Fagron	Biotin	17k20-B03-351524	1
Fagron	Biotin	17K20-B03-351524	1
Fagron	Biotin	19E22-B01-363404	1
Fagron	Biotin	20110634	1
Fagron	Biotin	20K09-F02-375271	1
Fagron	Biotin	20K09-F02-375272	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Biotin	22C02-B01-217682	1
Fagron	Biotin	F03-3775400	1
Fagron	Biotin	UE01704007	1
Fagron	Biotin	UE01807006	1
Fagron	Biotin	UE02005010	1
Fagron	Biotin	UE02005015	1
Gatt-Koller	Biotin	1634211	1
kögl	Biotin	17315206	1
KÖGL	Biotin	17315212	1
privat	Biotin	20171208-05-100	1

- 235 944 spectra from 1515 *Apo-Ident* customers from a total of 49 199 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Biotin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Biotin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	710	0	201 374
Type C	0	123	0	235 944

The substance/substance group *Biotin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.1549 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 95.1220 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21221	21904	13.84	158.01
21632	21904	6.46	161.10
21904	21904	0.00	163.16
22855	22855	0.00	164.46
22901	21904	4.37	164.60
22902	21904	4.93	165.10
23029	23029	0.00	166.30
23063	23063	0.00	165.56
24694	23029	11.48	166.91
25536	25536	0.00	165.10

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Bismuth gallath, basic**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21252-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bismuth gallath, basic; Bismuthi subgallas

Special notes

When selecting the *Bismuth gallath, basic* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Bismuth gallath, basic	6	5	247

Second-stage model

For differentiation of the substance/substance group *Bismuth gallath, basic* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Bismuth gallath, basic* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	79.94	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Bismuth gallath, basic* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Bismuth gallath, basic*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Bismuth gallath, basic	13179105	21252	40	1412254
Caelo	Bismuth gallath, basic	13179105	21553	60	20130701
Caelo	Bismuth gallath, basic	170041	23359	40	20170214*
Caelo	Bismuth gallath, basic	17004102	23372	40	20170214
Caelo	Bismuth gallath, basic	20000903	25204	40	20200331*
Fagron	Bismuth gallath, basic	15B02-B04-309481	22597	40	20150226
Fagron	Bismuth gallath, basic	15J26-B02-317883	22598	40	20151102

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 300 spectra of 7 reference samples from the substance/substance group *Bismuth gallath, basic*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 662 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 230 spectra of 6 reference samples from the substance/substance group *Bismuth gallath, basic*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Bismuth gallath, basic	191063	24714	40
Caelo	Bismuth gallath, basic	21003110	25845	50
Fagron	Bismuth gallath, basic	16K17-B04-335597	23570	40
Fagron	Bismuth gallath, basic	19K28-B02-196432	25186	40
Fagron	Bismuth gallath, basic	22I21-B04-223756	26617	40
Fagron	Bismuth gallath, basic	22I21-B04-223756	26617SI	20

- 201 854 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 880 spectra from 445 *Apo-Ident* customers from 264 batches from the substance/substance group *Bismuth gallath, basic*.

- Among them are spectra of independent samples from 247 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Bismuth gallath, basic	2022003849	2
	Bismuth gallath, basic	2023001183	1
	Bismuth gallath, basic	202300183	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
	Bismuth gallath, basic	2023004222	1
	Bismuth gallath, basic	21003110005	1
	Bismuth gallath, basic	21003110009	1
	Bismuth gallath, basic	21003110010	2
	Bismuth gallath, basic	21003110013	1
	Bismuth gallath, basic	21003110015	1
	Bismuth gallath, basic	21003110017	1
	Bismuth gallath, basic	21G21-B03-213570	2
	Bismuth gallath, basic	22I21-B04-228625	1
	Bismuth gallath, basic	22121-B04-228625	1
	Bismuth gallath, basic	B04-2286205	3
5N Plus GmbH / Ebert	Bismuth gallath, basic	18040801	1
5N Plus GmbH/Phoenix	Bismuth gallath, basic	2020000872	1
ahd/lamotte	Bismuth gallath, basic	13718_b13_292058	1
Alliance H.	Bismuth gallath, basic	15080602	1
Alliance Healthcare	Bismuth gallath, basic	13D19-N02	2
Alliance	Bismuth gallath, basic	12172402	1
Allianz Healthcare	Bismuth gallath, basic	15200911	1
Allianz Healthcare	Bismuth gallath, basic	17259517	1
Anzag	Bismuth gallath, basic	2012000059	2
apomix	Bismuth gallath, basic	13D19-N02	1
Bombastus	Bismuth gallath, basic	13/18-B13-292058	1
Bombastus	Bismuth gallath, basic	13G10-N12	1
Caelo	Bismuth gallath, basic		1
Caelo	Bismuth gallath, basic	10135109	1
Caelo	Bismuth gallath, basic	10D23-N05	1
Caelo	Bismuth gallath, basic	11127101	1
Caelo	Bismuth gallath, basic	11127104	1
Caelo	Bismuth gallath, basic	1127203	1
Caelo	Bismuth gallath, basic	12166901	2
Caelo	Bismuth gallath, basic	1217240	1
Caelo	Bismuth gallath, basic	12172401	1
Caelo	Bismuth gallath, basic	12172402	4
Caelo	Bismuth gallath, basic	12172409	6
Caelo	Bismuth gallath, basic	12172412	5
Caelo	Bismuth gallath, basic	12c13-n03	1
Caelo	Bismuth gallath, basic	12C13-N03	1
Caelo	Bismuth gallath, basic	12c13-no3	1
Caelo	Bismuth gallath, basic	12E16-N03	1
Caelo	Bismuth gallath, basic	12I13-N11	1
Caelo	Bismuth gallath, basic	13/18-B13-292057	1
Caelo	Bismuth gallath, basic	13/18-B13-292058	1
Caelo	Bismuth gallath, basic	13179101	2
Caelo	Bismuth gallath, basic	13179105	1
Caelo	Bismuth gallath, basic	13179111	6
Caelo	Bismuth gallath, basic	13D19-N02	2
Caelo	Bismuth gallath, basic	13I18-B13	1
Caelo	Bismuth gallath, basic	13I18-B13-294108	2
Caelo	Bismuth gallath, basic	14224103	4
Caelo	Bismuth gallath, basic	14224105	2
Caelo	Bismuth gallath, basic	15080602	3
Caelo	Bismuth gallath, basic	15080603	1
Caelo	Bismuth gallath, basic	15080606	10
Caelo	Bismuth gallath, basic	15200904	3
Caelo	Bismuth gallath, basic	15200905	1
Caelo	Bismuth gallath, basic	15200907	1
Caelo	Bismuth gallath, basic	15200910	2
Caelo	Bismuth gallath, basic	15200911	7
Caelo	Bismuth gallath, basic	15200913	4
Caelo	Bismuth gallath, basic	1520910	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Bismuth gallath, basic	1520913	1
Caelo	Bismuth gallath, basic	15B02-B04-304408	1
Caelo	Bismuth gallath, basic	15B02B04304413	1
Caelo	Bismuth gallath, basic	15B02-B04-309481	2
Caelo	Bismuth gallath, basic	15J26_B02-321313	1
Caelo	Bismuth gallath, basic	15J26-B02-320473	1
Caelo	Bismuth gallath, basic	15J26-B02-320479	1
Caelo	Bismuth gallath, basic	1603810	1
Caelo	Bismuth gallath, basic	16038308	7
Caelo	Bismuth gallath, basic	16038310	7
Caelo	Bismuth gallath, basic	16038312	9
Caelo	Bismuth gallath, basic	16K17-B04-335597	1
Caelo	Bismuth gallath, basic	17/26-B01-340556	1
Caelo	Bismuth gallath, basic	17004102	10
Caelo	Bismuth gallath, basic	17004106	10
Caelo	Bismuth gallath, basic	17004107	5
Caelo	Bismuth gallath, basic	17004109	9
Caelo	Bismuth gallath, basic	17004112	11
Caelo	Bismuth gallath, basic	1725909	1
Caelo	Bismuth gallath, basic	17259503	2
Caelo	Bismuth gallath, basic	17259505	4
Caelo	Bismuth gallath, basic	17259509	6
Caelo	Bismuth gallath, basic	17259510	6
Caelo	Bismuth gallath, basic	17259513	5
Caelo	Bismuth gallath, basic	17259517	7
Caelo	Bismuth gallath, basic	17259519	3
Caelo	Bismuth gallath, basic	17E16-B02-336992	1
Caelo	Bismuth gallath, basic	17-E16-B02-336992	1
Caelo	Bismuth gallath, basic	17I26-B01-341866	1
Caelo	Bismuth gallath, basic	18040801	11
Caelo	Bismuth gallath, basic	18A29-B06	1
Caelo	Bismuth gallath, basic	18A29-B06-346305	2
Caelo	Bismuth gallath, basic	18A29-B346305	1
Caelo	Bismuth gallath, basic	191063002	21
Caelo	Bismuth gallath, basic	191063004	6
Caelo	Bismuth gallath, basic	191063005	1
Caelo	Bismuth gallath, basic	191063006	8
Caelo	Bismuth gallath, basic	19106301	8
Caelo	Bismuth gallath, basic	19106302	6
Caelo	Bismuth gallath, basic	19B05-B09-191019	1
Caelo	Bismuth gallath, basic	20004232001	4
Caelo	Bismuth gallath, basic	20004232002	2
Caelo	Bismuth gallath, basic	20004232004	3
Caelo	Bismuth gallath, basic	2004232006	1
Caelo	Bismuth gallath, basic	2012006724	1
Caelo	Bismuth gallath, basic	2017002570	1
Caelo	Bismuth gallath, basic	21000126001	5
Caelo	Bismuth gallath, basic	21003110002	7
Caelo	Bismuth gallath, basic	21003110005	3
Caelo	Bismuth gallath, basic	21003110006	6
Caelo	Bismuth gallath, basic	21003110009	2
Caelo	Bismuth gallath, basic	21003110010	2
Caelo	Bismuth gallath, basic	21003110013	1
Caelo	Bismuth gallath, basic	220511(21000126001)	1
Caelo	Bismuth gallath, basic	23121410	1
Caelo	Bismuth gallath, basic	2414E-01185	1
Caelo	Bismuth gallath, basic	26011903	1
Caelo	Bismuth gallath, basic	5208I-01185	1
Caelo	Bismuth gallath, basic	62183516	1
Caelo	Bismuth gallath, basic	81297468	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Bismuth gallath, basic	8129768	1
Caelo	Bismuth gallath, basic	9205701	1
Caelo	Bismuth gallath, basic	9205703	2
Caelo	Bismuth gallath, basic	92057409	1
Caelo	Bismuth gallath, basic	9K26-N10	2
Caelo	Bismuth gallath, basic	B02-1964302	2
Caelo	Bismuth gallath, basic	B-150513-1	1
Caesar & Loretz GmbH…	Bismuth gallath, basic	17259505	1
Caesar & Loretz GmbH/Gehe	Bismuth gallath, basic	17259509	1
Caesar & Loretz GmbH/Gehe	Bismuth gallath, basic	191063006	1
Caesar & Loretz GmbH/Gehe	Bismuth gallath, basic	19106301	1
Caesar & Loretz GmbH/Gehe	Bismuth gallath, basic	21000126001	2
Caesar & Loretz GmbH…	Bismuth gallath, basic	20004232004	1
Caesar & Loretz GmbH…	Bismuth gallath, basic	191063006	1
Caesar & Loretz GmbH	Bismuth gallath, basic	16038312	2
Caesar & Loretz GmbH	Bismuth gallath, basic	17004102	1
Caesar & Loretz GmbH	Bismuth gallath, basic	17259509	2
Caesar & Loretz GmbH	Bismuth gallath, basic	17259510	2
Caesar & Loretz GmbH	Bismuth gallath, basic	17259513	3
Caesar & Loretz GmbH	Bismuth gallath, basic	191063002	4
Caesar & Loretz GmbH	Bismuth gallath, basic	191063004	4
Caesar & Loretz GmbH	Bismuth gallath, basic	191063006	6
Caesar & Loretz GmbH	Bismuth gallath, basic	19106301	3
Caesar & Loretz GmbH	Bismuth gallath, basic	20004232001	3
Caesar & Loretz GmbH	Bismuth gallath, basic	20004232004	2
Caesar & Loretz GmbH	Bismuth gallath, basic	21000126001	5
Caesar & Loretz GmbH	Bismuth gallath, basic	21003110002	5
Caesar & Loretz GmbH	Bismuth gallath, basic	21003110006	8
Caesar & Loretz GmbH	Bismuth gallath, basic	21003110009	1
Caesar/Ebert	Bismuth gallath, basic	17259509	1
Euro OTC	Bismuth gallath, basic	16K17-B04-335597	3
Fagro/Gehe	Bismuth gallath, basic	2018005145	1
Fagron	Bismuth gallath, basic		3
Fagron	Bismuth gallath, basic	10H31-N01	1
Fagron	Bismuth gallath, basic	114101-0003	1
Fagron	Bismuth gallath, basic	11F15-N03	1
Fagron	Bismuth gallath, basic	12/13-N11	1
Fagron	Bismuth gallath, basic	12B02-B04-304408	1
Fagron	Bismuth gallath, basic	12C13-N03	4
Fagron	Bismuth gallath, basic	12E16-N03	1
Fagron	Bismuth gallath, basic	12K26-N01	3
Fagron	Bismuth gallath, basic	13/18-B13-292057	2
Fagron	Bismuth gallath, basic	13/18-B-13-292057	1
Fagron	Bismuth gallath, basic	13/18-B13-292058	3
Fagron	Bismuth gallath, basic	13/18-B13294098	1
Fagron	Bismuth gallath, basic	13/18-B13-294098	2
Fagron	Bismuth gallath, basic	13/18-B13-294108	3
Fagron	Bismuth gallath, basic	13179111	1
Fagron	Bismuth gallath, basic	1318-B13-292057	2
Fagron	Bismuth gallath, basic	1318b13292058	1
Fagron	Bismuth gallath, basic	1318B1329409	1
Fagron	Bismuth gallath, basic	1318B13294108	1
Fagron	Bismuth gallath, basic	13D19-N02	3
Fagron	Bismuth gallath, basic	13E21-N03	2
Fagron	Bismuth gallath, basic	13F10-N12	1
Fagron	Bismuth gallath, basic	13G10-N12	4
Fagron	Bismuth gallath, basic	13I18-B13	5
Fagron	Bismuth gallath, basic	13I18-b13-292057	1
Fagron	Bismuth gallath, basic	13I18-B13-292057	2
Fagron	Bismuth gallath, basic	13I18-B13-292058	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Bismuth gallath, basic	13I18-B13-294098	4
Fagron	Bismuth gallath, basic	13i18-b13-294108	1
Fagron	Bismuth gallath, basic	13I18-B13-294108	6
Fagron	Bismuth gallath, basic	13K08-N03	4
Fagron	Bismuth gallath, basic	14H13-B07	1
Fagron	Bismuth gallath, basic	14H13B07303639	1
Fagron	Bismuth gallath, basic	14H13-B07-303639	6
Fagron	Bismuth gallath, basic	15/26-B02-320473	1
Fagron	Bismuth gallath, basic	15/26-B02-321313	1
Fagron	Bismuth gallath, basic	15126-B02-321313	1
Fagron	Bismuth gallath, basic	15B02-B04	3
Fagron	Bismuth gallath, basic	15B02-B04-209481	1
Fagron	Bismuth gallath, basic	15b02b04304408	1
Fagron	Bismuth gallath, basic	15B02-B04-304408	9
Fagron	Bismuth gallath, basic	15B02-B04-304413	5
Fagron	Bismuth gallath, basic	15b02-B04-309481	1
Fagron	Bismuth gallath, basic	15B02B04309481	1
Fagron	Bismuth gallath, basic	15B02-B04-309481	4
Fagron	Bismuth gallath, basic	15B02-B04-311878	1
Fagron	Bismuth gallath, basic	15C27-B02-311879	1
Fagron	Bismuth gallath, basic	15H05-B07	1
Fagron	Bismuth gallath, basic	15H05-B07-311880	5
Fagron	Bismuth gallath, basic	15I26-B02-325472	1
Fagron	Bismuth gallath, basic	15J26-B02	5
Fagron	Bismuth gallath, basic	15J26-B022	1
Fagron	Bismuth gallath, basic	15J26-B02-317883	9
Fagron	Bismuth gallath, basic	15J26-B02-320473	5
Fagron	Bismuth gallath, basic	15j26-b02-321313	1
Fagron	Bismuth gallath, basic	15J26-B02-321313	6
Fagron	Bismuth gallath, basic	15J26-B02-325450	1
Fagron	Bismuth gallath, basic	15J26-B02-325472	9
Fagron	Bismuth gallath, basic	15J26-BO2-321313	2
Fagron	Bismuth gallath, basic	16K17B04	1
Fagron	Bismuth gallath, basic	16K17-B04	1
Fagron	Bismuth gallath, basic	16K17-B04-3355593	1
Fagron	Bismuth gallath, basic	16K17B04335597	2
Fagron	Bismuth gallath, basic	16K17-B04-335597	11
Fagron	Bismuth gallath, basic	17/26-B01-340556	4
Fagron	Bismuth gallath, basic	17/26-B01-341866	1
Fagron	Bismuth gallath, basic	1726B01341866	1
Fagron	Bismuth gallath, basic	17E16-B02	4
Fagron	Bismuth gallath, basic	17E16-B02-336968	1
Fagron	Bismuth gallath, basic	17E16-B02-336992	3
Fagron	Bismuth gallath, basic	17G06-B10-355772	1
Fagron	Bismuth gallath, basic	17i26-B01	1
Fagron	Bismuth gallath, basic	17I26-B01-340552	4
Fagron	Bismuth gallath, basic	17I26-B01-340556	6
Fagron	Bismuth gallath, basic	17I26-B01-341866	5
Fagron	Bismuth gallath, basic	180307BB/2016006984	1
Fagron	Bismuth gallath, basic	180808186	1
Fagron	Bismuth gallath, basic	18A29-B06	2
Fagron	Bismuth gallath, basic	18A29-B06-3460303	1
Fagron	Bismuth gallath, basic	18A29-B06-346303	1
Fagron	Bismuth gallath, basic	18A29B06-346305	1
Fagron	Bismuth gallath, basic	18A29-B06-346305	8
Fagron	Bismuth gallath, basic	18A29-BO6-346305	1
Fagron	Bismuth gallath, basic	18G06-B10	2
Fagron	Bismuth gallath, basic	18G06-B10-352463	4
Fagron	Bismuth gallath, basic	18G06-B10-352486	3
Fagron	Bismuth gallath, basic	18G06-B10-353902	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Bismuth gallath, basic	18G06-B10-353916	6
Fagron	Bismuth gallath, basic	18G06B10355772	2
Fagron	Bismuth gallath, basic	18G06-B10-355772	6
Fagron	Bismuth gallath, basic	18K29-B06-346303	1
Fagron	Bismuth gallath, basic	191022	1
Fagron	Bismuth gallath, basic	19B05-B09-191019	4
Fagron	Bismuth gallath, basic	19B05-B09-191022	8
Fagron	Bismuth gallath, basic	19k28-B02	1
Fagron	Bismuth gallath, basic	19K28-B02	4
Fagron	Bismuth gallath, basic	19K28-B02-196431	12
Fagron	Bismuth gallath, basic	19k28b02196432	1
Fagron	Bismuth gallath, basic	19K28-B02-196432	18
Fagron	Bismuth gallath, basic	19k28-B02-201353	1
Fagron	Bismuth gallath, basic	19K28-B02-201353	2
Fagron	Bismuth gallath, basic	19K28Bo2-196432	1
Fagron	Bismuth gallath, basic	2010002685	2
Fagron	Bismuth gallath, basic	20114b10202382	1
Fagron	Bismuth gallath, basic	2012000059	3
Fagron	Bismuth gallath, basic	2012006724	2
Fagron	Bismuth gallath, basic	2013006220	1
Fagron	Bismuth gallath, basic	2014006082	1
Fagron	Bismuth gallath, basic	2015000361	3
Fagron	Bismuth gallath, basic	2015000866	1
Fagron	Bismuth gallath, basic	2015007568	4
Fagron	Bismuth gallath, basic	2016006984	1
Fagron	Bismuth gallath, basic	2017002570	1
Fagron	Bismuth gallath, basic	2017006945	4
Fagron	Bismuth gallath, basic	2018000237	2
Fagron	Bismuth gallath, basic	2018005145	7
Fagron	Bismuth gallath, basic	2019001542	11
Fagron	Bismuth gallath, basic	2020004951	2
Fagron	Bismuth gallath, basic	2021001320	1
Fagron	Bismuth gallath, basic	20I14_B10-202382	1
Fagron	Bismuth gallath, basic	20I14-B10	1
Fagron	Bismuth gallath, basic	20i14-B10-2023802	1
Fagron	Bismuth gallath, basic	20I14-B10-202382	4
Fagron	Bismuth gallath, basic	21F11-B99	2
Fagron	Bismuth gallath, basic	21F11-B99-215303	1
Fagron	Bismuth gallath, basic	21f11-b99-215304	1
Fagron	Bismuth gallath, basic	21F11-B99-215304	5
Fagron	Bismuth gallath, basic	21G21-B03	2
Fagron	Bismuth gallath, basic	21g21b0321213570	1
Fagron	Bismuth gallath, basic	21G21-B03-213244	1
Fagron	Bismuth gallath, basic	21G21-B03-213570	8
Fagron	Bismuth gallath, basic	21G21-B03-215370	1
Fagron	Bismuth gallath, basic	22121-B04-223756	1
Fagron	Bismuth gallath, basic	22I21-B04-223683	1
Fagron	Bismuth gallath, basic	22I21-B04-223756	2
Fagron	Bismuth gallath, basic	22l21-B04-223756	1
Fagron	Bismuth gallath, basic	26-B01-340552	1
Fagron	Bismuth gallath, basic	325472	1
Fagron	Bismuth gallath, basic	411092-3-P	1
Fagron	Bismuth gallath, basic	5121	1
Fagron	Bismuth gallath, basic	B02-1964302	1
Fagron	Bismuth gallath, basic	B02-2013503	1
Fagron	Bismuth gallath, basic	B02-201353	1
Fagron	Bismuth gallath, basic	b03-2135700	1
Fagron	Bismuth gallath, basic	B09-1910109	2
Fagron	Bismuth gallath, basic	B10-2023802	1
Fagron	Bismuth gallath, basic	BO2-1964302	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Bismuth gallath, basic	B03-2135700	1
Fargon GmbH & Co.KG	Bismuth gallath, basic	15J26-B02-321313	2
Fargon/ Noweda	Bismuth gallath, basic	15B02-B04-309481	1
Fargon/ Sanacorp	Bismuth gallath, basic	19K28-B02-196432	1
Fargon/Sanacorp	Bismuth gallath, basic	18A29-B06-346305	1
Fargon	Bismuth gallath, basic	13/18-B13-294108	1
Fargron	Bismuth gallath, basic	13D19-N02	1
Fargron	Bismuth gallath, basic	16k17-b04-335597	1
Frago/Noweda	Bismuth gallath, basic	16K17-B04-335597	1
Fragon/Sanacorp	Bismuth gallath, basic	16K17-B04-335593	1
Fragon/Sanacorp	Bismuth gallath, basic	17/26-B01-340552	1
Fragon/Sanacorp	Bismuth gallath, basic	18A-29-B06-346303	1
Fragon	Bismuth gallath, basic	19B05-B09-191022	1
Fragon	Bismuth gallath, basic	19K28-B02-19643	1
Fragon	Bismuth gallath, basic	19K28-B02-1964301	1
Fragon	Bismuth gallath, basic	19K28-B02-196431	2
Fragon	Bismuth gallath, basic	19K28-B02-196432	1
Gehe amax	Bismuth gallath, basic	15J26-B02-325450	1
Gehe	Bismuth gallath, basic	12172401	1
Gehe	Bismuth gallath, basic	15080607	1
Gehe	Bismuth gallath, basic	15J26-B02-317883	1
GEHE	Bismuth gallath, basic	17259509	1
Gehe	Bismuth gallath, basic	17E16-B02-336992	1
GEHE	Bismuth gallath, basic	18040801	1
GEHE	Bismuth gallath, basic	18A29-B06	2
Gehe	Bismuth gallath, basic	2015007568	1
Hedinger	Bismuth gallath, basic	16038310	1
Infectopharm	Bismuth gallath, basic	14224103	1
Kehr	Bismuth gallath, basic	17I26-B01-341866	1
Klenk	Bismuth gallath, basic	12E16-N03	1
L12	Bismuth gallath, basic	16038308	1
Martinus Apotheke	Bismuth gallath, basic	keine	1
Noweda	Bismuth gallath, basic	17/26-B01-341866	1
Noweda	Bismuth gallath, basic	18A29-B06-346303	1
Noweda	Bismuth gallath, basic	19K28-B02-196431	1
Noweda	Bismuth gallath, basic	19K28-B02-196432	1
Noweda	Bismuth gallath, basic	19K28-B02-201353	1
Noweda	Bismuth gallath, basic	20004232001	1
Noweda	Bismuth gallath, basic	21003110010	1
PHOENIX am 17.01.2014	Bismuth gallath, basic	2012006724	1
Phoenix, Jembke	Bismuth gallath, basic	10135101	1
Phoenix	Bismuth gallath, basic	1520913	1
Phoenix	Bismuth gallath, basic	191063002	1
Phönix	Bismuth gallath, basic	12-13-N11	1
Phönix	Bismuth gallath, basic	12E16-N03	1
phönix	Bismuth gallath, basic	15J26-B02-325450	1
Phönix	Bismuth gallath, basic	17259505	2
Phönix	Bismuth gallath, basic	19K28-B02	1
Phönix	Bismuth gallath, basic	19K28-B02-196432	1
Phönix	Bismuth gallath, basic	21g21-b03-213570	1
Sanacorp 03.01.22 23,00EUR	Bismuth gallath, basic	220103BE	1
Sanacorp 28.06.2017 ...	Bismuth gallath, basic	2015007568	1
Sanacorp	Bismuth gallath, basic	12/13-N11	1
sanacorp	Bismuth gallath, basic	13/1818B13-292057	1
Sanacorp	Bismuth gallath, basic	13D19-N02	1
Sanacorp	Bismuth gallath, basic	18A29-B06-346305	1
Sanacorp	Bismuth gallath, basic	19K28-B02-2013503	1
Sanacorp	Bismuth gallath, basic	2018005145	1
Sanacorp	Bismuth gallath, basic	2019001542-B02-201353	1
Sanacorp	Bismuth gallath, basic	B02-2013503	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sidonia	Bismuth gallath, basic	15200904	1
Sidonia	Bismuth gallath, basic	15J-26-B02-325450	1
Sidonia	Bismuth gallath, basic	17004107	3
siehe WE-Prüfprotokoll	Bismuth gallath, basic	4/09	1

- 235 187 spectra from 1515 *Apo-Ident* customers from a total of 48 995 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Bismuth gallath, basic* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bismuth gallath, basic* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	230	0	201 854
Type C	0	877	3	235 187

The substance/substance group *Bismuth gallath, basic* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.3913 %)
Type C	100.0000 % (> 99.9007 %)	99.6591 % (> 99.3182 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21252	21252	0.00	71.55
21553	21252	5.91	70.37

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22597	25204	10.31	68.73
22598	25204	9.59	69.22
23359	23359	0.00	70.71
23372	21252	9.39	68.13
25204	25204	0.00	70.98

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Boric acid**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20182-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Boric acid; Acidum boricum

Special notes

When selecting the *Boric acid* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Boric acid	6	5	44

Second-stage model

For differentiation of the substance/substance group *Boric acid* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Boric acid* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	93.46	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Boric acid* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Boric acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Boric acid	14133119	21804	60	20140509
Caelo	Boric acid	15425112	22964	40	20160104
Caelo	Boric acid	170613	23286	40	20170316*
Caelo	Boric acid	193010	25210	40	20200113*
Fagron	Boric acid	13I04-N06	21228	40	20130920
Fagron	Boric acid	15L09-B07-322988	23746	40	20151222

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 6 reference samples from the substance/substance group *Boric acid*. These

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 6 reference samples from the substance/substance group *Boric acid*.
- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Boric acid	15242903	22965	40
Caelo	Boric acid	191943	24741	40
Caelo	Boric acid	21001289	25698	50
Caelo	Boric acid	21000784	25701	50
Caelo	Boric acid	24001235	27258	40
Caelo	Boric acid	24001235	27258SI	20

- 201 844 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 81 spectra from 57 *Apo-Ident* customers from 49 batches from the substance/substance group *Boric acid*.
- Among them are spectra of independent samples from 44 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Boric acid	10227913	1
Caelo	Boric acid	11D13-N08	1
Caelo	Boric acid	12238901	1
Caelo	Boric acid	12260502	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Boric acid	14095202	1
Caelo	Boric acid	14133113	2
Caelo	Boric acid	14133119	1
Caelo	Boric acid	15095103	2
Caelo	Boric acid	15158901	1
Caelo	Boric acid	15158903	1
Caelo	Boric acid	15242906	1
Caelo	Boric acid	15242909	1
Caelo	Boric acid	15425101	5
Caelo	Boric acid	15425108	2
Caelo	Boric acid	15425112	2
Caelo	Boric acid	15425114	2
Caelo	Boric acid	15425118	3
Caelo	Boric acid	16291001	1
Caelo	Boric acid	17327901	4
Caelo	Boric acid	17327907	5
Caelo	Boric acid	17327912	2
Caelo	Boric acid	17327917	3
Caelo	Boric acid	193010003	1
Caelo	Boric acid	19301003	1
Caelo	Boric acid	20000508002	2
Caelo	Boric acid	20000508005	2
Caelo	Boric acid	200041/5001	1
Caelo	Boric acid	20004175001	1
Caelo	Boric acid	21000784001	1
Caelo	Boric acid	5425114	1
Caelo	Boric acid	80303AB	1
Caelo	Boric acid	9324021	1
Caelo	Boric acid	9324036	1
Caelo	Boric acid	9324043	1
Caesar & Loretz GmbH…	Boric acid	20000508002	1
Caesar & Loretz GmbH/Kehr	Boric acid	17327916	1
Caesar & Loretz GmbH	Boric acid	17327912	2
Caesar & Loretz GmbH	Boric acid	17327916	1
Caesar & Loretz GmbH	Boric acid	19194301	1
Caesar & Loretz GmbH	Boric acid	20000508002	2
Caesar & Loretz GmbH	Boric acid	20004175001	1
E Plus	Boric acid	15425108	1
Fagron	Boric acid	11d13-n08	1
Fagron	Boric acid	11I26-n05	1
Fagron	Boric acid	12f01-n08	1
Fagron	Boric acid	12G04-N10	1
Fagron	Boric acid	13A21-N06	1
Fagron	Boric acid	13I04-N06	2
Fagron	Boric acid	14133101	1
Fagron	Boric acid	14B07-B02-295752	1
Fagron	Boric acid	9082012B	1
Gatt-Koller	Boric acid	1803542	1
Labor	Boric acid	159095	1
Nachprüfung	Boric acid		1
Sanacorp	Boric acid	1/AKD3	1

- 235 986 spectra from 1515 *Apo-Ident* customers from a total of 49 210 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Boric acid* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Boric acid* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	240	0	201 844
Type C	0	81	0	235 986

The substance/substance group *Boric acid* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 92.5926 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21228	25210	10.83	167.63
21804	25210	3.85	165.22
22964	23286	15.58	179.31
23286	23286	0.00	199.91
23746	25210	9.94	169.42
25210	25210	0.00	171.74

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Budesonide**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20569-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Budesonide; Budesonidum

Special notes

When selecting the *Budesonide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Budesonide	8	13	186

Second-stage model

For differentiation of the substance/substance group *Budesonide* the following second-stage model is used:

- Submodel 07

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Budesonide* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prednisolon dihydrogen phosphate di…	72.92	–
⋮	⋮	⋮
Betamethasone valerate	>50	20.70
Erythromycin	>50	34.26

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Budesonide* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Budesonide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Budesonide	11351704	20808	40	AR-15-FG-005286-01
Caelo	Budesonide	161431	22627	40	20160606*
Caelo	Budesonide	161431	22627SI	25	20160606*
Caelo	Budesonide	15344004	22649	40	20151116
Caelo	Budesonide	15344004	22649SI	23	20151116
Euro OTC	Budesonide	1311022-01	21620	60	20140113
Euro OTC	Budesonide	1311022-01	21620SI	37	20140113
Euro OTC	Budesonide	1604018	22537	40	20160509*
Euro OTC	Budesonide	1604018	22537SI	23	20160509*
Euro OTC	Budesonide	2010006	25475	40	20201202*
Fagron	Budesonide	16J04-B01-326581	22841	40	20161026
Fagron	Budesonide	16J04-B01-326581	22888	40	20161026
Fagron	Budesonide	16J04-B01-326581	22888SI	30	20161026
Fagron	Budesonide	18C15-B03-355399	24699	40	20180409

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 518 spectra of 14 reference samples from the substance/substance group *Budesonide*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 444 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1021 spectra of 30 reference samples from the substance/substance group *Budesonide*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Budesonide	170788	23279	40
Caelo	Budesonide	180749	24026	40
Caelo	Budesonide	191381	24737	40
Caelo	Budesonide	20002391	25636	30
Caelo	Budesonide	23000636	26710	40
Euro OTC	Budesonide	1709022	23778	40
Euro OTC	Budesonide	1904004	24619	40
Euro OTC	Budesonide	2003043	25251	40
Euro OTC	Budesonide	2103025	25690	50
Euro OTC	Budesonide	2203005	26088	40
Euro OTC	Budesonide	2301044	26590	30
Euro OTC	Budesonide	2402017	27150	40
Fagron	Budesonide	22A12-B01-213702	26378	40
Caelo	Budesonide	15344004	22649SI†	7
Caelo	Budesonide	170788	23279SI	20
Caelo	Budesonide	180749	24026SI	20
Caelo	Budesonide	191381	24737SI	24
Caelo	Budesonide	20002391	25636SI	30
Caelo	Budesonide	23000636	26710SI	30
Euro OTC	Budesonide	1709022	23778SI	20

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Budesonide	1904004	24619SI	40
Euro OTC	Budesonide	2003043	25251SI	40
Euro OTC	Budesonide	2010006	25475SI†	39
Euro OTC	Budesonide	2103025	25690SI	50
Euro OTC	Budesonide	2203005	26088SI	40
Euro OTC	Budesonide	2301044	26590SI	32
Euro OTC	Budesonide	2402017	27150SI	30
Fagron	Budesonide	16J04-B01-326581	22841SI†	24
Fagron	Budesonide	18C15-B03-355399	24699SI†	35
Fagron	Budesonide	22A12-B01-213702	26378SI	30

- 201 063 spectra from a total of 4028 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 869 spectra from 256 *Apo-Ident* customers from 194 batches from the substance/substance group *Budesonide*.
- Among them are spectra of independent samples from 186 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Budesonide	20004092009	1
	Budesonide	20004092016	1
	Budesonide	20004092018	1
	Budesonide	20004092024	2
	Budesonide	20004092026	3
	Budesonide	21I20-B03-215349	1
	Budesonide	22A12-B01-228674	1
	Budesonide	23000636001	3
	Budesonide	23000636003	7
	Budesonide	23000636009	1
	Budesonide	23000636010	1
Anzag	Budesonide	19138101	1
Anzag	Budesonide	19138102	2
Bombastus	Budesonide	21100M1A0021321	1
Caelo	Budesonide	10061705	1
Caelo	Budesonide	11175014	2
Caelo	Budesonide	11175015	1
Caelo	Budesonide	11351701	1
Caelo	Budesonide	11351703	1
Caelo	Budesonide	11351706	5
Caelo	Budesonide	11351707	3
Caelo	Budesonide	11351713	1
Caelo	Budesonide	12295103	1
Caelo	Budesonide	12295105	1
Caelo	Budesonide	12295106	2

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Budesonide	12295108	1
Caelo	Budesonide	12295109	2
Caelo	Budesonide	12295110	4
Caelo	Budesonide	12295111	5
Caelo	Budesonide	1407116	1
Caelo	Budesonide	140711707	1
Caelo	Budesonide	14071701	2
Caelo	Budesonide	14071702	6
Caelo	Budesonide	14071706	1
Caelo	Budesonide	14071707	4
Caelo	Budesonide	14071713	1
Caelo	Budesonide	14071714	6
Caelo	Budesonide	14071716	2
Caelo	Budesonide	14071717	3
Caelo	Budesonide	1471707	1
Caelo	Budesonide	15044002	1
Caelo	Budesonide	15173802	4
Caelo	Budesonide	15173803	6
Caelo	Budesonide	15173804	3
Caelo	Budesonide	15173806	4
Caelo	Budesonide	15173807	3
Caelo	Budesonide	15173810	1
Caelo	Budesonide	15173811	8
Caelo	Budesonide	15344002	4
Caelo	Budesonide	15344003	7
Caelo	Budesonide	15344004	1
Caelo	Budesonide	15344005	4
Caelo	Budesonide	15344006	4
Caelo	Budesonide	15344008	8
Caelo	Budesonide	15344009	2
Caelo	Budesonide	15344010	3
Caelo	Budesonide	15344012	4
Caelo	Budesonide	15344013	1
Caelo	Budesonide	15344014	1
Caelo	Budesonide	16143101	7
Caelo	Budesonide	16143102	2
Caelo	Budesonide	16143103	3
Caelo	Budesonide	16143105	2
Caelo	Budesonide	16143106	3
Caelo	Budesonide	16143107	5
Caelo	Budesonide	16143108	10
Caelo	Budesonide	16143110	2
Caelo	Budesonide	16143112	2
Caelo	Budesonide	170078801	1
Caelo	Budesonide	170078808	1
Caelo	Budesonide	17078801	17
Caelo	Budesonide	17078803	3
Caelo	Budesonide	17078804	7
Caelo	Budesonide	17078805	16
Caelo	Budesonide	17078808	9
Caelo	Budesonide	17078809	6
Caelo	Budesonide	1709022	1
Caelo	Budesonide	17342902	5
Caelo	Budesonide	18074901	5
Caelo	Budesonide	18074902	11
Caelo	Budesonide	18074903	11
Caelo	Budesonide	18074905	11
Caelo	Budesonide	18074907	10
Caelo	Budesonide	18074908	11
Caelo	Budesonide	18074909	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Budesonide	181720608	1
Caelo	Budesonide	18172601	3
Caelo	Budesonide	18172603	14
Caelo	Budesonide	18172604	19
Caelo	Budesonide	18172606	6
Caelo	Budesonide	18172607	13
Caelo	Budesonide	18172608	8
Caelo	Budesonide	18172609	5
Caelo	Budesonide	18172610	3
Caelo	Budesonide	18172611	11
Caelo	Budesonide	18172614	4
Caelo	Budesonide	191381002	3
Caelo	Budesonide	191381004	13
Caelo	Budesonide	191381005	2
Caelo	Budesonide	19138101	22
Caelo	Budesonide	19138101P-200511-1	1
Caelo	Budesonide	19138101P-200709-1	1
Caelo	Budesonide	19138101P-200727-2	1
Caelo	Budesonide	19138102	27
Caelo	Budesonide	19138103	10
Caelo	Budesonide	200004092007	1
Caelo	Budesonide	200004092016	1
Caelo	Budesonide	20001092012	1
Caelo	Budesonide	2000402008	2
Caelo	Budesonide	20004092001	4
Caelo	Budesonide	20004092002	2
Caelo	Budesonide	20004092003	6
Caelo	Budesonide	20004092005	7
Caelo	Budesonide	20004092006	5
Caelo	Budesonide	20004092007	11
Caelo	Budesonide	20004092008	4
Caelo	Budesonide	20004092009	9
Caelo	Budesonide	20004092011	5
Caelo	Budesonide	20004092012	2
Caelo	Budesonide	20004092013	3
Caelo	Budesonide	20004092014	1
Caelo	Budesonide	20004092015	5
Caelo	Budesonide	20004092016	1
Caelo	Budesonide	20004092017	1
Caelo	Budesonide	20004092018	2
Caelo	Budesonide	20004092019	1
Caelo	Budesonide	20004092022	6
Caelo	Budesonide	20004092023	2
Caelo	Budesonide	20004092024	1
Caelo	Budesonide	20004092026	3
Caelo	Budesonide	20004092028	1
Caelo	Budesonide	20i17-f07-374500	1
Caelo	Budesonide	21100M1	1
Caelo	Budesonide	23000636003	1
Caelo	Budesonide	774865	1
Caelo	Budesonide	B-240619-2	1
Caelo	Budesonide	ChB14071717	1
Caeolo ,	Budesonide	17078809	1
Caesar & Lorenz GmbH	Budesonide	18172607	1
Caesar & Loretz GmbH...	Budesonide	191381002	1
Caesar & Loretz GmbH...	Budesonide	20004092002	1
Caesar & Loretz GmbH...	Budesonide	19138102	2
Caesar & Loretz GmbH...	Budesonide	19138101	1
Caesar & Loretz GmbH...	Budesonide	19138102	1
Caesar & Loretz GmbH...	Budesonide	20004092003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Budesonide	20004092018	1
Caesar & Loretz GmbH/Gehe	Budesonide	18172607	1
Caesar & Loretz GmbH/Gehe	Budesonide	20004092001	1
Caesar & Loretz GmbH/Gehe	Budesonide	20004092003	1
Caesar & Loretz GmbH/Gehe	Budesonide	20004092008	2
Caesar & Loretz GmbH/Gehe	Budesonide	20004092009	1
Caesar & Loretz GmbH/Gehe	Budesonide	20004092014	1
Caesar & Loretz GmbH...	Budesonide	191381002	1
Caesar & Loretz GmbH...	Budesonide	19138102	1
Caesar & Loretz GmbH...	Budesonide	20004092003	1
Caesar & Loretz GmbH...	Budesonide	20004092006	1
Caesar & Loretz GmbH...	Budesonide	19138102	1
Caesar & Loretz GmbH...	Budesonide	18172606	1
Caesar & Loretz GmbH/Sana	Budesonide	18172610	1
Caesar & Loretz GmbH...	Budesonide	18172603	1
Caesar & Loretz GmbH...	Budesonide	20004092009	1
Caesar & Loretz GmbH	Budesonide	17078808	1
Caesar & Loretz GmbH	Budesonide	17342902	1
Caesar & Loretz GmbH	Budesonide	18074905	1
Caesar & Loretz GmbH	Budesonide	18172603	1
Caesar & Loretz GmbH	Budesonide	18172604	2
Caesar & Loretz GmbH	Budesonide	18172606	5
Caesar & Loretz GmbH	Budesonide	18172608	6
Caesar & Loretz GmbH	Budesonide	18172610	1
Caesar & Loretz GmbH	Budesonide	18172611	3
Caesar & Loretz GmbH	Budesonide	18172614	2
Caesar & Loretz GmbH	Budesonide	1913810	1
Caesar & Loretz GmbH	Budesonide	191381002	8
Caesar & Loretz GmbH	Budesonide	191381004	3
Caesar & Loretz GmbH	Budesonide	191381005	3
Caesar & Loretz GmbH	Budesonide	19138101	11
Caesar & Loretz GmbH	Budesonide	19138102	12
Caesar & Loretz GmbH	Budesonide	19138103	8
Caesar & Loretz GmbH	Budesonide	2000402007	1
Caesar & Loretz GmbH	Budesonide	20004092001	1
Caesar & Loretz GmbH	Budesonide	20004092002	5
Caesar & Loretz GmbH	Budesonide	20004092003	2
Caesar & Loretz GmbH	Budesonide	20004092005	2
Caesar & Loretz GmbH	Budesonide	20004092006	2
Caesar & Loretz GmbH	Budesonide	20004092007	7
Caesar & Loretz GmbH	Budesonide	20004092008	4
Caesar & Loretz GmbH	Budesonide	20004092011	2
Caesar & Loretz GmbH	Budesonide	20004092012	3
Caesar & Loretz GmbH	Budesonide	20004092013	1
Caesar & Loretz GmbH	Budesonide	20004092015	2
Caesar & Loretz GmbH	Budesonide	20004092017	3
Caesar & Loretz GmbH	Budesonide	20004092018	3
Caesar & Loretz GmbH	Budesonide	20004092019	1
Caesar & Loretz GmbH	Budesonide	20004092022	1
Caesar & Loretz GmbH	Budesonide	20004092024	3
Cealo / Otto Geilenk...	Budesonide	19138101	1
Cealo/Gehe	Budesonide	19138103	1
Cealo/Sanacorp	Budesonide	20004092006	1
Cealo	Budesonide	17078804	1
Ceolo/Spangro	Budesonide	191381002	1
crystal pharma/gehe	Budesonide	1305004-01	2
Euro OTC	Budesonide	1311022-01	5
Euro OTC	Budesonide	1604018-01	2
Euro OTC	Budesonide	1709022-01	2
Euro OTC	Budesonide	1709022-02	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Budesonide	18172609	1
Euro OTC	Budesonide	1904004-01	2
Euro OTC	Budesonide	2203005-01	1
Euro OTC	Budesonide	709022-02	1
Fagron	Budesonide		2
Fagron	Budesonide	12D03-N03	1
Fagron	Budesonide	12G23-N01	2
Fagron	Budesonide	13A07-N09	1
Fagron	Budesonide	13H22-N03	2
Fagron	Budesonide	14A30-B09_291366	1
Fagron	Budesonide	14A30-B09-291366	2
Fagron	Budesonide	14H15-B02	3
Fagron	Budesonide	14H15-B02-297926	1
Fagron	Budesonide	14H15-B02-301971	2
Fagron	Budesonide	14H15-B02-301972	1
Fagron	Budesonide	15344012	1
Fagron	Budesonide	15E27_B10	1
Fagron	Budesonide	15E27-B01-308321	1
Fagron	Budesonide	15e27-b10-308321	1
Fagron	Budesonide	15E27-B10-308321	1
Fagron	Budesonide	15e27-b10-308322	1
Fagron	Budesonide	15E27-B10-308322	1
Fagron	Budesonide	15E27-B10-315704	1
Fagron	Budesonide	16J04-B01	1
Fagron	Budesonide	16j04-b01-326583	3
Fagron	Budesonide	17a17-b01	1
Fagron	Budesonide	17A17-B01	1
Fagron	Budesonide	17A17-B01-331248	1
Fagron	Budesonide	17A17-B01-331448	4
Fagron	Budesonide	17F28-B04-345016	2
Fagron	Budesonide	18074901	1
Fagron	Budesonide	18172601	1
Fagron	Budesonide	18C15-B03-350266	4
Fagron	Budesonide	18C15-B03-353058	2
Fagron	Budesonide	18C15-B03-355399	3
Fagron	Budesonide	19/27-F02-366343	1
Fagron	Budesonide	19F06-B06	2
Fagron	Budesonide	19f06-B06-363444	1
Fagron	Budesonide	19F06-B06-363447	1
Fagron	Budesonide	19F-06-B06-363447	1
Fagron	Budesonide	19I27-F02-366344	1
Fagron	Budesonide	1B001192001	1
Fagron	Budesonide	1B00119201	1
Fagron	Budesonide	1B003202001	2
Fagron	Budesonide	20/17-F07	1
Fagron	Budesonide	20G17-F03-372894	1
Fagron	Budesonide	20G17-F03-372894	1
Fagron	Budesonide	20I17-F07	1
Fagron	Budesonide	20I17-F07-374499	2
Fagron	Budesonide	20l17-F07-374500	1
Fagron	Budesonide	21b05_b17-213703	1
Fagron	Budesonide	21B05-B17	1
Fagron	Budesonide	21I20-B03-215348	1
Fagron	Budesonide	21I20-B03-215664	1
Fagron	Budesonide	21l20-B03-215664	1
Fagron	Budesonide	C2280092	1
Fargon/Kehr	Budesonide	16J04-B01-326583	1
Farmabios/Noweda	Budesonide	21100M1B0031821	2
Farmabios/Phoenix	Budesonide	21100M1B0021821	1
Gehe	Budesonide	14071714	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Budesonide	16143103	1
Gehe	Budesonide	16143107	1
Gehe	Budesonide	17078801	1
GEHE	Budesonide	18074901	1
Gehe	Budesonide	18074902	3
GEHE	Budesonide	18172601	2
Gehe	Budesonide	18172604	1
Gehe	Budesonide	20004092024	1
Geibo/ Fargron	Budesonide	15E27-B10-315704	1
Geibo/ Fargron	Budesonide	17A17-b01-331448	1
Jenne	Budesonide	20004092024	1
L10	Budesonide	15344012	1
Noweda/Caesar & Lore...	Budesonide	19138101	1
Noweda	Budesonide	1604018-01	1
Noweda	Budesonide	16143108	1
Noweda	Budesonide	16143110	1
Noweda	Budesonide	17078803	1
Noweda	Budesonide	18074903	1
Noweda	Budesonide	18172608	1
Noweda	Budesonide	191381004	1
Noweda	Budesonide	20004092012	1
Noweda	Budesonide	20004092022	1
Noweda	Budesonide	20004092028	1
Noweda	Budesonide	23000636001	2
Otto Geilenkirchen	Budesonide	23000636003	1
Phoenix	Budesonide	14071702	3
Phoenix	Budesonide	15344013	1
phoenix	Budesonide	19138103	1
Phoenix	Budesonide	23000636009	1
Phönix	Budesonide	18074907	1
Phönix	Budesonide	18172607	1
Phönix	Budesonide	191381004	1
Sanacorp /Fargron	Budesonide	17A17-B01-331448	1
Sanacorp,	Budesonide	16143103	1
sanacorp	Budesonide	14071701	1
Sanacorp	Budesonide	17078801	1
Sanacorp	Budesonide	17078805	1
Sanacorp	Budesonide	18074902	1
Sanacorp	Budesonide	18074907	1
sanacorp	Budesonide	191381004	1
Sanacorp	Budesonide	20004092024	1
Sanacorp	Budesonide	20004092029	1
Sanacorp	Budesonide	23000636003	1
Sanacorp	Budesonide	23000636004	1
VDl 23.10.14 19,50 euro	Budesonide	14071707	1

- 235 198 spectra from 1515 *Apo-Ident* customers from a total of 49 068 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Budesonide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Budesonide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table

breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	518	0	152 444
Type B	0	1021	0	201 063
Type C	0	820	49	235 198

The substance/substance group *Budesonide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8417 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4123 %)
Type C	100.0000 % (> 99.9007 %)	94.3613 % (> 94.0161 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20808	20808	0.00	139.72
21620	20808	5.23	131.19
22537	22537	0.00	116.23
22627	22627	0.00	121.71
22649	22537	7.87	119.24
22841	22627	4.41	122.54
22888	22627	7.99	122.90
24699	25475	8.11	120.73
25475	25475	0.00	124.81

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Bupivacaine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	24435-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Bupivacaine hydrochloride; Bupivacaini hydrochloridum

Special notes

When selecting the *Bupivacaine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Bupivacaine hydrochloride	3	1	0

Second-stage model

For differentiation of the substance/substance group *Bupivacaine hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Bupivacaine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	86.52	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Bupivacaine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Bupivacaine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Bupivacaine hydrochloride	17E22-B08-345817	24435	40	1905513
Fagron	Bupivacaine hydrochloride	21J11-B06-219298	26464	40	20211202
Fagron	Bupivacaine hydrochloride	23A04-B09-233749	27026	40	20230209
Fagron	Bupivacaine hydrochloride	23A04-B09-233749	27026SI	20	20230209

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 140 spectra of 4 reference samples from the substance/substance group *Bupivacaine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 152 822 spectra from a total of 2839 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 60 spectra of 2 reference samples from the substance/substance group *Bupivacaine hydrochloride*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Bupivacaine hydrochloride	17L05-B04-358735	24594	40
Fagron	Bupivacaine hydrochloride	21J11-B06-219298	26464SI†	20

- 202 024 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Bupivacaine hydrochloride*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Bupivacaine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Bupivacaine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	140	0	152 822
Type B	0	55	5	202 024
Type C	0	0	0	236 067

The substance/substance group *Bupivacaine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9912 %)	91.6667 % (> 86.6667 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24435	24435	0.00	208.72
26464	24435	56.19	198.02
27026	24435	20.54	205.97

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Butylated hydroxytoluene**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21307-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Butylated hydroxytoluene; Butylhydroxytoluenum

Special notes

When selecting the *Butylated hydroxytoluene* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Butylated hydroxytoluene	6	4	82

Second-stage model

For differentiation of the substance/substance group *Butylated hydroxytoluene* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Butylated hydroxytoluene* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prednisolon dihydrogen phosphate di…	103.01	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Butylated hydroxytoluene* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Butylated hydroxytoluene*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Butylated hydroxytoluene	13354602	21307	40	20131105
Caelo	Butylated hydroxytoluene	13354604	21355	40	AR-15-FG-007846-02
Caelo	Butylated hydroxytoluene	15172103	21911	60	20150529
Caelo	Butylated hydroxytoluene	15172103	22281	60	20150529
Caelo	Butylated hydroxytoluene	15172103	22350	60	20150529
Caelo	Butylated hydroxytoluene	190749	24554	40	20190405*
Caelo	Butylated hydroxytoluene	20000734	25552	40	20200324*
Caelo	Butylated hydroxytoluene	23000635	27322	40	20230503*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 380 spectra of 8 reference samples from the substance/substance group *Butylated hydroxytoluene*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 582 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 210 spectra of 7 reference samples from the substance/substance group *Butylated hydroxytoluene*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Butylated hydroxytoluene	163163	23356	40
Caelo	Butylated hydroxytoluene	180291	24019	40
Caelo	Butylated hydroxytoluene	21004127	25999	40
Caelo	Butylated hydroxytoluene	24002119	27440	40
Caelo	Butylated hydroxytoluene	21004127	25999SI	10
Caelo	Butylated hydroxytoluene	23000635	27322SI†	20
Caelo	Butylated hydroxytoluene	24002119	27440SI	20

- 201 874 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 834 spectra from 539 *Apo-Ident* customers from 85 batches from the substance/substance group *Butylated hydroxytoluene*.

- Among them are spectra of independent samples from 82 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Butylated hydroxytoluene	16316304	1
	Butylated hydroxytoluene	21004127001	2
	Butylated hydroxytoluene	22002085003	11
	Butylated hydroxytoluene	23000635001	7
	Butylated hydroxytoluene	23001370001	1
AHC	Butylated hydroxytoluene	23000635001	1
AHD	Butylated hydroxytoluene	18029102	1
Allianz Healthcare	Butylated hydroxytoluene	19074902	1
Apo Ident/ Noweda	Butylated hydroxytoluene	18029104	1
Bombastus	Butylated hydroxytoluene	13354604	1
Caelo	Butylated hydroxytoluene	11(18029107)	1
Caelo	Butylated hydroxytoluene	11131006	1
Caelo	Butylated hydroxytoluene	12(20000734001)	1
Caelo	Butylated hydroxytoluene	12158201	3
Caelo	Butylated hydroxytoluene	12158204	5
Caelo	Butylated hydroxytoluene	12207005	3
Caelo	Butylated hydroxytoluene	1220705	1
Caelo	Butylated hydroxytoluene	122080206	1
Caelo	Butylated hydroxytoluene	12280201	2
Caelo	Butylated hydroxytoluene	12280203	5
Caelo	Butylated hydroxytoluene	12280206	4
Caelo	Butylated hydroxytoluene	123823	1
Caelo	Butylated hydroxytoluene	12382302	5
Caelo	Butylated hydroxytoluene	12382304	7
Caelo	Butylated hydroxytoluene	12382307	1
Caelo	Butylated hydroxytoluene	12382309	8
Caelo	Butylated hydroxytoluene	12382312	1
Caelo	Butylated hydroxytoluene	13354602	4
Caelo	Butylated hydroxytoluene	13354604	8
Caelo	Butylated hydroxytoluene	13354609	2
Caelo	Butylated hydroxytoluene	13354611	4
Caelo	Butylated hydroxytoluene	1400501	1
Caelo	Butylated hydroxytoluene	1426801	1
Caelo	Butylated hydroxytoluene	143004502	1
Caelo	Butylated hydroxytoluene	14300501	11
Caelo	Butylated hydroxytoluene	14300502	8
Caelo	Butylated hydroxytoluene	14300503	2
Caelo	Butylated hydroxytoluene	14300505	6
Caelo	Butylated hydroxytoluene	14300506	2
Caelo	Butylated hydroxytoluene	15094501	12
Caelo	Butylated hydroxytoluene	15172101	11
Caelo	Butylated hydroxytoluene	15172103	21
Caelo	Butylated hydroxytoluene	15172105	12
Caelo	Butylated hydroxytoluene	15426801	13
Caelo	Butylated hydroxytoluene	1542680118029105	1
Caelo	Butylated hydroxytoluene	15426807	17
Caelo	Butylated hydroxytoluene	1631301	1
Caelo	Butylated hydroxytoluene	1631601	1
Caelo	Butylated hydroxytoluene	16316301	23
Caelo	Butylated hydroxytoluene	16316304	19
Caelo	Butylated hydroxytoluene	16316304-20180619Ma5	1
Caelo	Butylated hydroxytoluene	16316305	16
Caelo	Butylated hydroxytoluene	163163055402	1
Caelo	Butylated hydroxytoluene	16316307	29
Caelo	Butylated hydroxytoluene	18029102	22
Caelo	Butylated hydroxytoluene	18029104	8
Caelo	Butylated hydroxytoluene	18029105	44
Caelo	Butylated hydroxytoluene	18029107	24
Caelo	Butylated hydroxytoluene	18029108	13
Caelo	Butylated hydroxytoluene	1802915	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Butylated hydroxytoluene	18048701	20
Caelo	Butylated hydroxytoluene	18229102	1
Caelo	Butylated hydroxytoluene	190749001	39
Caelo	Butylated hydroxytoluene	19074901	19
Caelo	Butylated hydroxytoluene	19074902	27
Caelo	Butylated hydroxytoluene	20000734001	26
Caelo	Butylated hydroxytoluene	2000734001	2
Caelo	Butylated hydroxytoluene	20161112-1	1
Caelo	Butylated hydroxytoluene	21000037001	40
Caelo	Butylated hydroxytoluene	21000037004	5
Caelo	Butylated hydroxytoluene	2100037001	1
Caelo	Butylated hydroxytoluene	21004127001	25
Caelo	Butylated hydroxytoluene	21004127002	9
Caelo	Butylated hydroxytoluene	2100427001	1
Caelo	Butylated hydroxytoluene	2113U02851	1
Caelo	Butylated hydroxytoluene	2170717	1
Caelo	Butylated hydroxytoluene	22002082001	1
Caelo	Butylated hydroxytoluene	22002085001	1
Caelo	Butylated hydroxytoluene	22002085003	4
Caelo	Butylated hydroxytoluene	220804(21004127001)	1
Caelo	Butylated hydroxytoluene	23000635001	1
Caelo	Butylated hydroxytoluene	231115BHT	1
Caelo	Butylated hydroxytoluene	2749	1
Caelo	Butylated hydroxytoluene	5426807	1
Caelo	Butylated hydroxytoluene	6316301	1
Caelo	Butylated hydroxytoluene	7031403	1
Caelo	Butylated hydroxytoluene	716M-02851	1
Caelo	Butylated hydroxytoluene	BT28112013	1
Caesar & Loretz /Gehe	Butylated hydroxytoluene	19074902	1
Caesar & Loretz GmbH...	Butylated hydroxytoluene	18029105	1
Caesar & Loretz GmbH...	Butylated hydroxytoluene	21000037001	1
Caesar & Loretz GmbH...	Butylated hydroxytoluene	190749001	1
Caesar & Loretz GmbH...	Butylated hydroxytoluene	18029108	1
Caesar & Loretz GmbH...	Butylated hydroxytoluene	18029107	1
Caesar & Loretz GmbH...	Butylated hydroxytoluene	21000037001	1
Caesar & Loretz GmbH...	Butylated hydroxytoluene	21000037004	1
Caesar & Loretz GmbH/AHD	Butylated hydroxytoluene	19074902	1
Caesar & Loretz GmbH/AHD	Butylated hydroxytoluene	21000037004	1
Caesar & Loretz GmbH/Gehe	Butylated hydroxytoluene	19074902	2
Caesar & Loretz GmbH/GEHE	Butylated hydroxytoluene	19074902	1
Caesar & Loretz GmbH/Gehe	Butylated hydroxytoluene	21000037001	1
Caesar & Loretz GmbH...	Butylated hydroxytoluene	190749001	1
Caesar & Loretz GmbH...	Butylated hydroxytoluene	19074902	1
Caesar & Loretz GmbH...	Butylated hydroxytoluene	21004127001	1
Caesar & Loretz GmbH...	Butylated hydroxytoluene	21004127001	2
Caesar & Loretz GmbH...	Butylated hydroxytoluene	21000037001	1
Caesar & Loretz GmbH...	Butylated hydroxytoluene	18029107	1
Caesar & Loretz GmbH...	Butylated hydroxytoluene	19074902	1
Caesar & Loretz GmbH...	Butylated hydroxytoluene	20000734001	1
Caesar & Loretz GmbH...	Butylated hydroxytoluene	21000037001	1
Caesar & Loretz GmbH...	Butylated hydroxytoluene	21004127002	1
Caesar & Loretz GmbH	Butylated hydroxytoluene	18029102	1
Caesar & Loretz GmbH	Butylated hydroxytoluene	18029105	4
Caesar & Loretz GmbH	Butylated hydroxytoluene	18029107	3
Caesar & Loretz GmbH	Butylated hydroxytoluene	18029108	3
Caesar & Loretz GmbH	Butylated hydroxytoluene	190749001	10
Caesar & Loretz GmbH	Butylated hydroxytoluene	19074901	9
Caesar & Loretz GmbH	Butylated hydroxytoluene	19074902	8
Caesar & Loretz GmbH	Butylated hydroxytoluene	20000734001	15
Caesar & Loretz GmbH	Butylated hydroxytoluene	21000037001	12

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Butylated hydroxytoluene	21000037004	6
Caesar & Loretz GmbH	Butylated hydroxytoluene	21004127001	12
Caesar & Loretz GmbH	Butylated hydroxytoluene	21004127002	7
Caesar & Loretz GmbH	Butylated hydroxytoluene	22002085001	1
Caesar & Loretz GmbH	Butylated hydroxytoluene	22002085003	3
Caesar & Loretz Hilden	Butylated hydroxytoluene	18029105	1
Caesar & Loretz/Noweda	Butylated hydroxytoluene	21000037001	1
Caesar & Loretz	Butylated hydroxytoluene	15426801	1
Caesar & Loretz	Butylated hydroxytoluene	16316307	1
Caesar Loretz	Butylated hydroxytoluene	190749001	1
Cealo / Otto Geilenk...	Butylated hydroxytoluene	18029108	1
Cealo/Sanacorp	Butylated hydroxytoluene	21004127001	1
Celo	Butylated hydroxytoluene	15426801	1
Euro OTC	Butylated hydroxytoluene	15172105	1
Euro OTC	Butylated hydroxytoluene	15426807	1
Euro OTC	Butylated hydroxytoluene	18029107	1
Fagron	Butylated hydroxytoluene	11308701	1
Fagron	Butylated hydroxytoluene	15426801	1
Fagron	Butylated hydroxytoluene	16316304	1
Fiebig	Butylated hydroxytoluene	15426807	1
Fiebig	Butylated hydroxytoluene	18029105	1
Gehe	Butylated hydroxytoluene	15426807	1
Gehe	Butylated hydroxytoluene	18029105	3
GEHE	Butylated hydroxytoluene	18029105	1
Gehe	Butylated hydroxytoluene	18029107	1
Gehe	Butylated hydroxytoluene	19074901	1
Gehe	Butylated hydroxytoluene	20000734001	2
Krieger	Butylated hydroxytoluene	16316301	1
Krieger	Butylated hydroxytoluene	18029108	1
L12	Butylated hydroxytoluene	15426807	1
L12	Butylated hydroxytoluene	16316307	1
Nachprüfung	Butylated hydroxytoluene	123456	1
Noweda	Butylated hydroxytoluene	12158201	1
Noweda	Butylated hydroxytoluene	12382304	1
Noweda	Butylated hydroxytoluene	15172103	1
Noweda	Butylated hydroxytoluene	15426807	1
Noweda	Butylated hydroxytoluene	16316305	1
Noweda	Butylated hydroxytoluene	18029105	2
Noweda	Butylated hydroxytoluene	21000037001	1
Noweda	Butylated hydroxytoluene	21004127002	1
Noweda	Butylated hydroxytoluene	23000635003	1
Phoenix	Butylated hydroxytoluene	12382305	1
Phoenix	Butylated hydroxytoluene	13354609	1
Phoenix	Butylated hydroxytoluene	15426801	1
Phoenix	Butylated hydroxytoluene	16316301	1
Phoenix	Butylated hydroxytoluene	20000734001	1
Phoenix	Butylated hydroxytoluene	21000037001	1
Phoenix	Butylated hydroxytoluene	22002085003	1
Phoenix	Butylated hydroxytoluene	3111201	1
Phönix/Caesar&Lorenz...	Butylated hydroxytoluene	22002085003	1
PHÖNIX	Butylated hydroxytoluene	16316304	1
Phönix	Butylated hydroxytoluene	16316307	1
Phönix	Butylated hydroxytoluene	18029102	1
Phönix	Butylated hydroxytoluene	190749001	1
Phönix	Butylated hydroxytoluene	19074901	1
PHÖNIX	Butylated hydroxytoluene	20000734001	1
Sanacorp	Butylated hydroxytoluene	13354609	1
Sanacorp	Butylated hydroxytoluene	14300505	1
sanacorp	Butylated hydroxytoluene	15172103	1
Sanacorp	Butylated hydroxytoluene	15172103	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Butylated hydroxytoluene	16316305	1
Sanacorp	Butylated hydroxytoluene	18029105	1
Sanacorp	Butylated hydroxytoluene	2100037004	1
Sanacorp	Butylated hydroxytoluene	22002085003	1
Sanacorp	Butylated hydroxytoluene	23000635001	1
SanacorpWE:04.01.18 …	Butylated hydroxytoluene	16316304	1

- 235 233 spectra from 1515 *Apo-Ident* customers from a total of 49 176 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Butylated hydroxytoluene* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Butylated hydroxytoluene* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	210	0	201 874
Type C	0	829	5	235 233

The substance/substance group *Butylated hydroxytoluene* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.1429 %)
Type C	100.0000 % (> 99.9007 %)	99.4005 % (> 99.0408 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21307	21355	7.82	236.32
21355	21355	0.00	241.73
21911	21355	9.17	240.81
22281	21355	6.03	245.70
22350	21355	7.06	241.16
24554	24554	0.00	254.17
25552	25552	0.00	244.97
27322	27322	0.00	251.43

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Caffeine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20962-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Caffeine; Coffeinum

Special notes

When selecting the *Caffeine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Caffeine	7	9	100

Second-stage model

For differentiation of the substance/substance group *Caffeine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Caffeine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Caffeine citrate	142.24	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Caffeine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Caffeine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Caffeine	12317911	21089	40	20121113
Caelo	Caffeine	12317911	21205	40	20121113
Caelo	Caffeine	13233105	21456	60	20131008
Caelo	Caffeine	13233104	21548	60	20131008
Euro OTC	Caffeine	1211012-01	20962	40	1412248
Euro OTC	Caffeine	1808017	24199	40	20180905*
Euro OTC	Caffeine	1909022	24980	40	20191022*
Fagron	Caffeine	22A19-B05-219102	26161	40	20220531

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 360 spectra of 8 reference samples from the substance/substance group *Caffeine*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 602 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 430 spectra of 12 reference samples from the substance/substance group *Caffeine*.

- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Caffeine	15082303	22823	40
Caelo	Caffeine	21001749	25798	50
Caelo	Caffeine	23000642	26711	40
Euro OTC	Caffeine	1603009	22517	40
Euro OTC	Caffeine	1703006	23140	40
Euro OTC	Caffeine	1907006	24784	40
Euro OTC	Caffeine	2001041	25079	40
Euro OTC	Caffeine	2205020	26201	40
Euro OTC	Caffeine	2311014	27068	40
Caelo	Caffeine	23000642	26711SI	20
Euro OTC	Caffeine	2205020	26201SI	20
Fagron	Caffeine	22A19-B05-219102	26161SI†	20

- 201 654 spectra from a total of 4035 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 470 spectra from 271 *Apo-Ident* customers from 105 batches from the substance/substance group *Caffeine*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 99 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Caffeine	20014041-02	1
	Caffeine	21052089	1
	Caffeine	22002096001	3
	Caffeine	22002096010	12
	Caffeine	2205020-01	1
	Caffeine	2205020-02	2
	Caffeine	2205020-03	4
	Caffeine	2205050-03	1
	Caffeine	23000642003	2
	Caffeine	2311014-01	2
ACM	Caffeine	KNC1294J14	2
AHD	Caffeine	2205020-03	1
Alliance Healthcare	Caffeine	18011928	1
apo-ident	Caffeine	1808017-01	1
Bombastus	Caffeine	1307049-01	1
Caelo	Caffeine	11076807	2
Caelo	Caffeine	11111111	1
Caelo	Caffeine	12093402	2
Caelo	Caffeine	12093410	2
Caelo	Caffeine	12093418	2
Caelo	Caffeine	1211012-01	1
Caelo	Caffeine	12317902	1
Caelo	Caffeine	12317904	2
Caelo	Caffeine	12317906	1
Caelo	Caffeine	12317909	8
Caelo	Caffeine	12317914	2
Caelo	Caffeine	13233105	4
Caelo	Caffeine	13233111	6
Caelo	Caffeine	1503020-01	2
Caelo	Caffeine	15054704	3
Caelo	Caffeine	15054709	3
Caelo	Caffeine	15082311	1
Caelo	Caffeine	15082315	1
Caelo	Caffeine	15372012	1
Caelo	Caffeine	15375006	4
Caelo	Caffeine	15375007	6
Caelo	Caffeine	15375012	6
Caelo	Caffeine	15375013	1
Caelo	Caffeine	1703006-01	4
Caelo	Caffeine	17133704	1
Caelo	Caffeine	17173704	10
Caelo	Caffeine	17173705	10
Caelo	Caffeine	17173707	5
Caelo	Caffeine	180119001	1
Caelo	Caffeine	180119002	3
Caelo	Caffeine	18011901	6
Caelo	Caffeine	18011902	6
Caelo	Caffeine	18011906	9
Caelo	Caffeine	18011911	38
Caelo	Caffeine	18011915	9
Caelo	Caffeine	18011920	14
Caelo	Caffeine	18011928	8
Caelo	Caffeine	180119911	1
Caelo	Caffeine	18077906	1
Caelo	Caffeine	1808017-01	1
Caelo	Caffeine	19000754002	13
Caelo	Caffeine	1907006-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Caffeine	21000088004	26
Caelo	Caffeine	21000088006	1
Caelo	Caffeine	21001749004	2
Caelo	Caffeine	21001749006	3
Caelo	Caffeine	21001749014	2
Caelo	Caffeine	21001749015	3
Caelo	Caffeine	22002096001	2
Caelo	Caffeine	3212E-01281	1
Caelo	Caffeine	9301807	1
Caesar & Lorenz	Caffeine	22002096001	1
Caesar & Loretz GmbH…	Caffeine	21001749002	1
Caesar & Loretz GmbH…	Caffeine	21001749004	1
Caesar & Loretz GmbH…	Caffeine	19000754002	3
Caesar & Loretz GmbH…	Caffeine	180119002	1
Caesar & Loretz GmbH	Caffeine	180119001	1
Caesar & Loretz GmbH	Caffeine	180119002	3
Caesar & Loretz GmbH	Caffeine	18011912	2
Caesar & Loretz GmbH	Caffeine	18011915	2
Caesar & Loretz GmbH	Caffeine	18011920	2
Caesar & Loretz GmbH	Caffeine	18011928	2
Caesar & Loretz GmbH	Caffeine	19000754002	4
Caesar & Loretz GmbH	Caffeine	21000088004	2
Caesar & Loretz GmbH	Caffeine	21000088006	2
Caesar & Loretz GmbH	Caffeine	21001749002	1
Caesar & Loretz GmbH	Caffeine	21001749004	1
Caesar & Loretz GmbH	Caffeine	21001749006	3
Caesar & Loretz GmbH	Caffeine	21001749014	1
Caesar & Loretz GmbH	Caffeine	21001749015	1
Caesar & Loretz GmbH	Caffeine	22002096001	1
Caesar&Loretz GmbH	Caffeine	21001749006	1
EuRho	Caffeine	17030006-02	2
EuRho	Caffeine	1808017-02	1
Euro OTC	Caffeine		1
Euro OTC	Caffeine	1109017-01	1
Euro OTC	Caffeine	1211012-01	1
Euro OTC	Caffeine	1211012-02	1
Euro OTC	Caffeine	1307049-01	4
Euro OTC	Caffeine	1404026-01	1
Euro OTC	Caffeine	1411015-01	4
Euro OTC	Caffeine	1503020-01	6
Euro OTC	Caffeine	1503020-02	8
Euro OTC	Caffeine	1603009/01	1
Euro OTC	Caffeine	160300901	2
Euro OTC	Caffeine	1603009-01	2
Euro OTC	Caffeine	1603009-02	4
Euro OTC	Caffeine	163009-01	1
Euro OTC	Caffeine	16462119	1
Euro OTC	Caffeine	1703006	1
Euro OTC	Caffeine	1703006-01	23
Euro OTC	Caffeine	1703006-02	9
Euro OTC	Caffeine	17173704	1
Euro OTC	Caffeine	1808017	3
Euro OTC	Caffeine	1808017_01	1
Euro OTC	Caffeine	1808017-01	7
Euro OTC	Caffeine	180801702	1
Euro OTC	Caffeine	1808017-02	3
Euro OTC	Caffeine	180881701	1
Euro OTC	Caffeine	1818017-02	1
Euro OTC	Caffeine	18212023	1
Euro OTC	Caffeine	18808017-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Caffeine	1907006-01	5
Euro OTC	Caffeine	1907006-1	1
Euro OTC	Caffeine	1909022-01	5
Euro OTC	Caffeine	2001041-01	3
Euro OTC	Caffeine	2001041-02	12
Euro OTC	Caffeine	2205020-01	1
Euro OTC	Caffeine	2205020-02	1
Euro OTC	Caffeine	26081406	1
Euro OTC	Caffeine	291001903	2
Euro OTC	Caffeine	31071701	1
Euro OTC	Caffeine	325241AX20	1
Euro OTC	Caffeine	5101701	1
EUro/AHD	Caffeine	121012-01	1
EUro/AHD	Caffeine	1307049-01	1
Euro/Noweda	Caffeine	1703006-01	1
Fagron	Caffeine	123456	1
Fagron	Caffeine	15H11-B02	1
Fagron	Caffeine	17173704	1
Gatt-Koller / Phoenix	Caffeine	5898/12135213	2
Gatt-Koller	Caffeine	1803747	1
Gehe	Caffeine	18011915	2
GEHE	Caffeine	22002096001	1
Gehe	Caffeine	23000642002	1
Gehe	Caffeine	23000642003	1
Klenk	Caffeine	1411015-01	1
Merck	Caffeine	MerckReagenziensatz	1
Noweda/Caesar & Lore…	Caffeine	21001749014	1
Noweda	Caffeine	1404026-01	1
Noweda	Caffeine	2001041-01	1
Phoenix	Caffeine	1808017-01	1
Phönix	Caffeine	1603009-02	1
Reagenz	Caffeine		1
Sanacorp	Caffeine		2
Sanacorp	Caffeine	19000754002	1
siegfried pharma che…	Caffeine	1909022-01	1
Siegfried PharmaChem…	Caffeine	1808017-01	1

- 235 597 spectra from 1515 *Apo-Ident* customers from a total of 49 156 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Caffeine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Caffeine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	430	0	201 654
Type C	0	458	12	235 597

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The substance/substance group *Caffeine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6047 %)
Type C	100.0000 % (> 99.9007 %)	97.4468 % (> 96.8085 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20962	20962	0.00	232.38
21089	24199	7.15	239.45
21205	24199	6.43	238.47
21456	24980	8.05	236.47
21548	20962	10.42	225.98
24199	24199	0.00	241.53
24980	24980	0.00	246.12
26161	24199	23.57	256.14

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Caffeine citrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20701-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Caffeine citrate; Coffeini citras

Special notes

When selecting the *Caffeine citrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Caffeine citrate	5	2	30

Second-stage model

For differentiation of the substance/substance group *Caffeine citrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Caffeine citrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	111.91	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Caffeine citrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Caffeine citrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Caffeine citrate	12C16-N03	20701	40	1403477
Fagron	Caffeine citrate	15A05-B03-318006	22530	40	20150115
Fagron	Caffeine citrate	15A05-B03-318006	22531	40	20150115
Gatt-Koller	Caffeine citrate	1783/05140715	21844	60	AR-15-FG-014994-01
Gatt-Koller	Caffeine citrate	22J00881	26626	40	20220718
Gatt-Koller	Caffeine citrate	23J02625	27092	40	20240130
Gatt-Koller	Caffeine citrate	23J02625	27092SI	20	20240130

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 7 reference samples from the substance/substance group *Caffeine citrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 682 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 4 reference samples from the substance/substance group *Caffeine citrate*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Caffeine citrate	15A05-B03-302746	21734	60
Gatt-Koller	Caffeine citrate	4065/11164916	23112	40
Fagron	Caffeine citrate	15A05-B03-302746	22729	40
Gatt-Koller	Caffeine citrate	22J00881	26626SI†	20

- 201 924 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 82 spectra from 55 *Apo-Ident* customers from 34 batches from the substance/substance group *Caffeine citrate*.
- Among them are spectra of independent samples from 30 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
AHD	Caffeine citrate	13B08-N02	1
Caelo	Caffeine citrate	11F21-N05	1
Caelo	Caffeine citrate	13D30-N02	1
Caelo	Caffeine citrate	15A05-B03-302746	1
Caelo	Caffeine citrate	15A05-B03-307309	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Caffeine citrate	15A05-B03-318006	2
Fagron	Caffeine citrate	10c23-n02	1
Fagron	Caffeine citrate	10H02-N02	2
Fagron	Caffeine citrate	11082015A	1
Fagron	Caffeine citrate	11C29-N04	2
Fagron	Caffeine citrate	12C16-N03	1
Fagron	Caffeine citrate	12J05-N06	3
Fagron	Caffeine citrate	12J05-N06	1
Fagron	Caffeine citrate	13B08N02	1
Fagron	Caffeine citrate	13B08-N02	1
Fagron	Caffeine citrate	13D30-N02	9
Fagron	Caffeine citrate	13D30-No2	1
Fagron	Caffeine citrate	15A05B03	1
Fagron	Caffeine citrate	15A05-B03	3
Fagron	Caffeine citrate	15a05-b03-302746	1
Fagron	Caffeine citrate	15A05-B03-302746	11
Fagron	Caffeine citrate	15A05-B03-307135	3
Fagron	Caffeine citrate	15a05-b03-318006	1
Fagron	Caffeine citrate	15A05-B03-318006	11
Fagron	Caffeine citrate	2002311282	1
Fagron	Caffeine citrate	204311282	1
Fagron	Caffeine citrate	26021401	1
Fagron	Caffeine citrate	2714E-01282	1
Fagron	Caffeine citrate	2813E1282	1
Fagron	Caffeine citrate	3314E-01282	1
Fagron	Caffeine citrate	3513I-01282	1
Fagron	Caffeine citrate	3914U-01282	1
Fagron	Caffeine citrate	4213U01282	1
Fagron	Caffeine citrate	5013U01282	1
Fagron	Caffeine citrate	CCC1205	1
Fagron	Caffeine citrate	CCD-1401	3
Fargon/Phoenix	Caffeine citrate	15A05-B03-302746	1
Fargon	Caffeine citrate	12J05-N06	1
Fgron	Caffeine citrate	2013Q-01282	1
Gehe	Caffeine citrate	13B08-N02	1
Noweda	Caffeine citrate	CCC-1101	1
Phoenix	Caffeine citrate	15A05-B03	1
Rondell Apotheke	Caffeine citrate	15A05-B03-307309	1

- 235 985 spectra from 1515 *Apo-Ident* customers from a total of 49 224 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Caffeine citrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Caffeine citrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	160	0	201 924
Type C	0	72	10	235 985

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The substance/substance group *Caffeine citrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	87.8049 % (> 84.1463 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20701	20701	0.00	342.93
21844	21844	0.00	279.24
22530	20701	24.26	343.26
22531	20701	29.21	343.94
26626	21844	102.51	262.52
27092	21844	100.50	292.99

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Calcium ascorbate dihydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20393-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Calcium ascorbate dihydrate; Calcii ascorbas dihydricum

Special notes

When selecting the *Calcium ascorbate dihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Calcium ascorbate dihydrate	9	14	18

Second-stage model

For differentiation of the substance/substance group *Calcium ascorbate dihydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Calcium ascorbate dihydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	84.23	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Calcium ascorbate dihydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Calcium ascorbate dihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Calcium ascorbate dihydrate	13105624	21313	40	20130620
Caelo	Calcium ascorbate dihydrate	163111	23060	40	20161207*
Caelo	Calcium ascorbate dihydrate	16311101	23518	40	20161207
Caelo	Calcium ascorbate dihydrate	20003812	25625	40	20201211*
Euro OTC	Calcium ascorbate dihydrate	1612003	22916	40	20170110*
Euro OTC	Calcium ascorbate dihydrate	1709005	23609	40	20170914*
Euro OTC	Calcium ascorbate dihydrate	1709004	23611	40	20170914*
Euro OTC	Calcium ascorbate dihydrate	1801010	23884	40	20180115*
Euro OTC	Calcium ascorbate dihydrate	2201040	26093	40	20220211*
Euro OTC	Calcium ascorbate dihydrate	2201040	26093SI	20	20220211*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 380 spectra of 10 reference samples from the substance/substance group *Calcium ascorbate dihydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 582 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 590 spectra of 16 reference samples from the substance/substance group *Calcium ascorbate dihydrate*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Calcium ascorbate dihydrate	183226	24373	40
Caelo	Calcium ascorbate dihydrate	19000538	25223	40
Caelo	Calcium ascorbate dihydrate	22000185	26014	30
Euro OTC	Calcium ascorbate dihydrate	1607033-01	22812	40
Euro OTC	Calcium ascorbate dihydrate	1807032	24194	40
Euro OTC	Calcium ascorbate dihydrate	1901003	24470	40
Euro OTC	Calcium ascorbate dihydrate	1904010	24626	40
Euro OTC	Calcium ascorbate dihydrate	1910003	24979	40
Euro OTC	Calcium ascorbate dihydrate	2003025	25149	40
Euro OTC	Calcium ascorbate dihydrate	2007012	25336	40
Euro OTC	Calcium ascorbate dihydrate	2101005	25538	40
Euro OTC	Calcium ascorbate dihydrate	2105006	25768	50
Euro OTC	Calcium ascorbate dihydrate	2305017	26881	40
Euro OTC	Calcium ascorbate dihydrate	2403007	27345	40
Caelo	Calcium ascorbate dihydrate	22000185	26014SI	10
Euro OTC	Calcium ascorbate dihydrate	2305017	26881SI	20

- 201 494 spectra from a total of 4031 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 28 spectra from 12 *Apo-Ident* customers from 21 batches from the substance/substance group *Calcium ascorbate dihydrate*.

- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Calcium ascorbate dihydrate	2305017-01	2
Arktis	Calcium ascorbate dihydrate	7339/4617	1
Arktis	Calcium ascorbate dihydrate	733P/1518	1
Burton Feingold	Calcium ascorbate dihydrate	L008415	1
Caelo	Calcium ascorbate dihydrate	13105608	1
Caelo	Calcium ascorbate dihydrate	14340907	1
Caelo	Calcium ascorbate dihydrate	15324702	1
Caelo	Calcium ascorbate dihydrate	15324708	2
Caelo	Calcium ascorbate dihydrate	16311101	1
Caelo	Calcium ascorbate dihydrate	16311105	1
Euro OTC	Calcium ascorbate dihydrate	1709004-01	1
Euro OTC	Calcium ascorbate dihydrate	1709005	1
Euro OTC	Calcium ascorbate dihydrate	1801010	1
Euro OTC	Calcium ascorbate dihydrate	1901003-01	1
Euro OTC	Calcium ascorbate dihydrate	1904010-01	3
Euro OTC	Calcium ascorbate dihydrate	1910003-01	3
Euro OTC	Calcium ascorbate dihydrate	2007012-01	2
Euro OTC	Calcium ascorbate dihydrate	2105006-01	1
Euro OTC	Calcium ascorbate dihydrate	220104001	1
Farmalabor / Farmalabor	Calcium ascorbate dihydrate	P1104931-000A	1
Gatt-Koller	Calcium ascorbate dihydrate	1900123	1

- 236 039 spectra from 1515 *Apo-Ident* customers from a total of 49 237 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Calcium ascorbate dihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Calcium ascorbate dihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	590	0	201 494
Type C	0	28	0	236 039

The substance/substance group *Calcium ascorbate dihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.9831 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 78.5714 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21313	23060	9.77	202.22
22916	22916	0.00	200.63
23060	23060	0.00	199.49
23518	25625	4.00	198.10
23609	23609	0.00	199.49
23611	23611	0.00	198.66
23884	23884	0.00	198.08
25625	25625	0.00	200.46
26093	26093	0.00	202.84

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Calcium citrate tetrahydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20013-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Calcium citrate tetrahydrate; Calcii citras tetrahydricus

Special notes

When selecting the *Calcium citrate tetrahydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Calcium citrate tetrahydrate	8	10	129

Second-stage model

For differentiation of the substance/substance group *Calcium citrate tetrahydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Calcium citrate tetrahydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	73.70	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Calcium citrate tetrahydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Calcium citrate tetrahydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Calcium citrate tetrahydrate	13391203	21320	40	20131205
Caelo	Calcium citrate tetrahydrate	13391203	21486	40	20131205
Caelo	Calcium citrate tetrahydrate	171768	23651	40	20170713*
Euro OTC	Calcium citrate tetrahydrate	1305018-01	21249	40	20130528
Euro OTC	Calcium citrate tetrahydrate	1509039	21931	60	20151013*
Euro OTC	Calcium citrate tetrahydrate	1509039-01	22255	60	20151013
Euro OTC	Calcium citrate tetrahydrate	1701001	22995	40	20170124*
Euro OTC	Calcium citrate tetrahydrate	2206009	26184	40	20220624*
Euro OTC	Calcium citrate tetrahydrate	2206009	26184SI	20	20220624*
Euro OTC	Calcium citrate tetrahydrate	2305020	26748	40	20230607*
Euro OTC	Calcium citrate tetrahydrate	2305020	26748SI	20	20230607*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 440 spectra of 11 reference samples from the substance/substance group *Calcium citrate tetrahydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 522 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 430 spectra of 11 reference samples from the substance/substance group *Calcium citrate tetrahydrate*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Calcium citrate tetrahydrate	181608	24230	40
Caelo	Calcium citrate tetrahydrate	20002273	25287	40
Caelo	Calcium citrate tetrahydrate	21004151	26124	40
Caelo	Calcium citrate tetrahydrate	24001206	27230	40
Euro OTC	Calcium citrate tetrahydrate	1606001	22681	40
Euro OTC	Calcium citrate tetrahydrate	1707025	23606	40
Euro OTC	Calcium citrate tetrahydrate	1803031	24077	40
Euro OTC	Calcium citrate tetrahydrate	1901002	24514	40
Euro OTC	Calcium citrate tetrahydrate	1912013	25075	40
Euro OTC	Calcium citrate tetrahydrate	2105004	25769	50
Caelo	Calcium citrate tetrahydrate	21004151	26124SI	20

- 201 654 spectra from a total of 4035 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 330 spectra from 146 *Apo-Ident* customers from 135 batches from the substance/substance group *Calcium citrate tetrahydrate*.

- Among them are spectra of independent samples from 129 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Calcium citrate tetrahydrate	21004151003	2
	Calcium citrate tetrahydrate	21004151004	1
	Calcium citrate tetrahydrate	21004151009	1
8,35Caesar & Loretz GmbH	Calcium citrate tetrahydrate	20002273013	1
ACM	Calcium citrate tetrahydrate	KNC0740J15	1
Alliance Health 23.1...	Calcium citrate tetrahydrate	1402003-01	1
Alliance Healthcare	Calcium citrate tetrahydrate	20002273006	2
Caelo	Calcium citrate tetrahydrate		2
Caelo	Calcium citrate tetrahydrate	11061402	1
Caelo	Calcium citrate tetrahydrate	11168803	1
Caelo	Calcium citrate tetrahydrate	11168806	3
Caelo	Calcium citrate tetrahydrate	11168813	1
Caelo	Calcium citrate tetrahydrate	1119E-01209	1
Caelo	Calcium citrate tetrahydrate	11349301	1
Caelo	Calcium citrate tetrahydrate	11349304	2
Caelo	Calcium citrate tetrahydrate	11349309	2
Caelo	Calcium citrate tetrahydrate	11349313	2
Caelo	Calcium citrate tetrahydrate	11349318	3
Caelo	Calcium citrate tetrahydrate	11349320	1
Caelo	Calcium citrate tetrahydrate	11349325	2
Caelo	Calcium citrate tetrahydrate	1168806	1
Caelo	Calcium citrate tetrahydrate	1168813	1
Caelo	Calcium citrate tetrahydrate	12310401	1
Caelo	Calcium citrate tetrahydrate	12310402	2
Caelo	Calcium citrate tetrahydrate	12310403	3
Caelo	Calcium citrate tetrahydrate	12310406	5
Caelo	Calcium citrate tetrahydrate	12310407	2
Caelo	Calcium citrate tetrahydrate	12310411	2
Caelo	Calcium citrate tetrahydrate	12310413	4
Caelo	Calcium citrate tetrahydrate	12310417	3
Caelo	Calcium citrate tetrahydrate	12310418	2
Caelo	Calcium citrate tetrahydrate	13391203	4
Caelo	Calcium citrate tetrahydrate	133912042x	1
Caelo	Calcium citrate tetrahydrate	13391205	5
Caelo	Calcium citrate tetrahydrate	1408017-01	1
Caelo	Calcium citrate tetrahydrate	14133303	1
Caelo	Calcium citrate tetrahydrate	14133307	1
Caelo	Calcium citrate tetrahydrate	14133310	1
Caelo	Calcium citrate tetrahydrate	1509039-01	1
Caelo	Calcium citrate tetrahydrate	1509039-02	1
Caelo	Calcium citrate tetrahydrate	15177701	1
Caelo	Calcium citrate tetrahydrate	15177702	2
Caelo	Calcium citrate tetrahydrate	15177703	7
Caelo	Calcium citrate tetrahydrate	15375702	6
Caelo	Calcium citrate tetrahydrate	15375703	1
Caelo	Calcium citrate tetrahydrate	15375707	1
Caelo	Calcium citrate tetrahydrate	15375712	2
Caelo	Calcium citrate tetrahydrate	15375713	6
Caelo	Calcium citrate tetrahydrate	1600565	1
Caelo	Calcium citrate tetrahydrate	16021502	1
Caelo	Calcium citrate tetrahydrate	16056501	1
Caelo	Calcium citrate tetrahydrate	16056504	4
Caelo	Calcium citrate tetrahydrate	16056505	3
Caelo	Calcium citrate tetrahydrate	16056510	2
Caelo	Calcium citrate tetrahydrate	1606001-02	1
Caelo	Calcium citrate tetrahydrate	1705038-01	1
Caelo	Calcium citrate tetrahydrate	1707025-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Calcium citrate tetrahydrate	1716803	1
Caelo	Calcium citrate tetrahydrate	1716808	1
Caelo	Calcium citrate tetrahydrate	17176803	6
Caelo	Calcium citrate tetrahydrate	17176805	1
Caelo	Calcium citrate tetrahydrate	17176806	6
Caelo	Calcium citrate tetrahydrate	17176808	7
Caelo	Calcium citrate tetrahydrate	17176812	3
Caelo	Calcium citrate tetrahydrate	17176816	1
Caelo	Calcium citrate tetrahydrate	17176818	1
Caelo	Calcium citrate tetrahydrate	18160802	3
Caelo	Calcium citrate tetrahydrate	18160803	1
Caelo	Calcium citrate tetrahydrate	18160805	1
Caelo	Calcium citrate tetrahydrate	18160811	1
Caelo	Calcium citrate tetrahydrate	18160813	2
Caelo	Calcium citrate tetrahydrate	19010002-01	1
Caelo	Calcium citrate tetrahydrate	19061315	1
Caelo	Calcium citrate tetrahydrate	20002273004	2
Caelo	Calcium citrate tetrahydrate	20002273009	2
Caelo	Calcium citrate tetrahydrate	20002273010	1
Caelo	Calcium citrate tetrahydrate	20002273013	2
Caelo	Calcium citrate tetrahydrate	2000227306	1
Caelo	Calcium citrate tetrahydrate	2001377004	1
Caelo	Calcium citrate tetrahydrate	2016Q-01209	1
Caelo	Calcium citrate tetrahydrate	21001377004	1
Caelo	Calcium citrate tetrahydrate	21004151002	1
Caelo	Calcium citrate tetrahydrate	2114M1209	1
Caelo	Calcium citrate tetrahydrate	3512U-01209	1
Caelo	Calcium citrate tetrahydrate	71356168	1
Caelo	Calcium citrate tetrahydrate	92192429	1
Caelo	Calcium citrate tetrahydrate	92457399	1
Caesar & Loretz GmbH...	Calcium citrate tetrahydrate	20002273013	1
Caesar & Loretz GmbH...	Calcium citrate tetrahydrate	18160811	1
Caesar & Loretz GmbH...	Calcium citrate tetrahydrate	181608002	3
Caesar & Loretz GmbH...	Calcium citrate tetrahydrate	21001377004	1
Caesar & Loretz GmbH...	Calcium citrate tetrahydrate	21004151002	2
Caesar & Loretz GmbH/OG	Calcium citrate tetrahydrate	20002273002	1
Caesar & Loretz GmbH...	Calcium citrate tetrahydrate	20002273010	1
Caesar & Loretz GmbH	Calcium citrate tetrahydrate	17176814	1
Caesar & Loretz GmbH	Calcium citrate tetrahydrate	181608002	3
Caesar & Loretz GmbH	Calcium citrate tetrahydrate	18160802	3
Caesar & Loretz GmbH	Calcium citrate tetrahydrate	18160804	3
Caesar & Loretz GmbH	Calcium citrate tetrahydrate	18160811	1
Caesar & Loretz GmbH	Calcium citrate tetrahydrate	18160812	3
Caesar & Loretz GmbH	Calcium citrate tetrahydrate	18160813	1
Caesar & Loretz GmbH	Calcium citrate tetrahydrate	20002273002	2
Caesar & Loretz GmbH	Calcium citrate tetrahydrate	20002273004	3
Caesar & Loretz GmbH	Calcium citrate tetrahydrate	20002273009	3
Caesar & Loretz GmbH	Calcium citrate tetrahydrate	20002273013	1
Caesar & Loretz GmbH	Calcium citrate tetrahydrate	21001377004	1
Caesar & Loretz GmbH	Calcium citrate tetrahydrate	21001377009	1
Caesar & Loretz	Calcium citrate tetrahydrate	16056509	1
Cealo	Calcium citrate tetrahydrate	12310401	1
Dr.Lohmann	Calcium citrate tetrahydrate	3042527	1
EuRho/Jenne	Calcium citrate tetrahydrate	1211007-01	1
EuRho	Calcium citrate tetrahydrate	1502012-02	1
euro ct	Calcium citrate tetrahydrate	1912013-01	5
Euro OTC	Calcium citrate tetrahydrate	1009030-01	1
Euro OTC	Calcium citrate tetrahydrate	1058904	1
Euro OTC	Calcium citrate tetrahydrate	1207006-01	2
Euro OTC	Calcium citrate tetrahydrate	1211007-01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Calcium citrate tetrahydrate	13031204	1
Euro OTC	Calcium citrate tetrahydrate	1305018-01	3
Euro OTC	Calcium citrate tetrahydrate	1305018-02	1
Euro OTC	Calcium citrate tetrahydrate	1402003-01	2
Euro OTC	Calcium citrate tetrahydrate	140801701	1
Euro OTC	Calcium citrate tetrahydrate	1408017-01	4
Euro OTC	Calcium citrate tetrahydrate	1502012-01	1
Euro OTC	Calcium citrate tetrahydrate	1502021-02	1
Euro OTC	Calcium citrate tetrahydrate	1509039-01	4
Euro OTC	Calcium citrate tetrahydrate	1509039-02	6
Euro OTC	Calcium citrate tetrahydrate	15177704	1
Euro OTC	Calcium citrate tetrahydrate	1606001-01	1
Euro OTC	Calcium citrate tetrahydrate	1606001-02	2
Euro OTC	Calcium citrate tetrahydrate	1701001-01	2
Euro OTC	Calcium citrate tetrahydrate	1701001-02	1
Euro OTC	Calcium citrate tetrahydrate	1707025-01	3
Euro OTC	Calcium citrate tetrahydrate	1707025-02	2
Euro OTC	Calcium citrate tetrahydrate	1707025-41	1
Euro OTC	Calcium citrate tetrahydrate	1710007-01	1
Euro OTC	Calcium citrate tetrahydrate	1803031-01	3
Euro OTC	Calcium citrate tetrahydrate	1803031-02	7
Euro OTC	Calcium citrate tetrahydrate	190100201	1
Euro OTC	Calcium citrate tetrahydrate	1901002-01	6
Euro OTC	Calcium citrate tetrahydrate	1901002-02	4
Euro OTC	Calcium citrate tetrahydrate	191201301	1
Euro OTC	Calcium citrate tetrahydrate	1912013-01	12
Euro OTC	Calcium citrate tetrahydrate	1912013-02	6
Euro OTC	Calcium citrate tetrahydrate	1912013-13	1
Euro OTC	Calcium citrate tetrahydrate	2105004-01	3
Euro OTC	Calcium citrate tetrahydrate	2817U-01209	1
Euro OTC	Calcium citrate tetrahydrate	3006222	1
Euro OTC	Calcium citrate tetrahydrate	3037086	1
Euro OTC	Calcium citrate tetrahydrate	3842527	1
Fagron	Calcium citrate tetrahydrate	13d16-n06	1
Fagron	Calcium citrate tetrahydrate	13D16-N06	1
Fagron	Calcium citrate tetrahydrate	150903901	1
Gatt-Koller	Calcium citrate tetrahydrate	1802139	3
Gehe Kassel	Calcium citrate tetrahydrate	14133307	1
Gehe	Calcium citrate tetrahydrate	18160806	1
Gehe	Calcium citrate tetrahydrate	21001377009	1
Krieger	Calcium citrate tetrahydrate	17176808	1
L12	Calcium citrate tetrahydrate	1606001-03	1
lohmann	Calcium citrate tetrahydrate	3045397	1
Noweda	Calcium citrate tetrahydrate	1509039-01	1
Noweda	Calcium citrate tetrahydrate	17176803	1
Noweda	Calcium citrate tetrahydrate	17176808	1
Noweda	Calcium citrate tetrahydrate	18160804	1
Noweda	Calcium citrate tetrahydrate	18160813	1
Noweda	Calcium citrate tetrahydrate	20002273004	1
Phönix	Calcium citrate tetrahydrate	1305018-01	1
Sanacorp WE: 12.08.1…	Calcium citrate tetrahydrate	711105	1
Sanacorp	Calcium citrate tetrahydrate	1211007-01	1
Sanacorp	Calcium citrate tetrahydrate	14133310	1
Sanacorp	Calcium citrate tetrahydrate	20002273002	1

- 235 737 spectra from 1515 *Apo-Ident* customers from a total of 49 126 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Calcium citrate tetrahydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Calcium citrate tetrahydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	430	0	201 654
Type C	0	330	0	235 737

The substance/substance group *Calcium citrate tetrahydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6047 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 98.1818 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21249	22995	6.17	101.73
21320	22995	7.49	105.13
21486	22995	7.26	105.83
21931	21931	0.00	96.86
22255	21931	4.74	97.82
22995	22995	0.00	101.06
23651	23651	0.00	101.68
26184	26184	0.00	101.99
26748	26748	0.00	101.93

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Calcium gluconate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20871-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Calcium gluconate; Calcii gluconas

Special notes

When selecting the *Calcium gluconate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Calcium gluconate	6	9	82

Second-stage model

For differentiation of the substance/substance group *Calcium gluconate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Calcium gluconate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	68.67	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Calcium gluconate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Calcium gluconate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Calcium gluconate	12236502	20871	40	1401575
Caelo	Calcium gluconate	12335829	21312	40	20121121
Euro OTC	Calcium gluconate	1304012-01	21283	40	AR-15-FG-008127-01
Euro OTC	Calcium gluconate	1407041-01	21821	60	20140818
Euro OTC	Calcium gluconate	1712007	23873	40	20171220*
Euro OTC	Calcium gluconate	1911017	25086	40	20200123*
Euro OTC	Calcium gluconate	1712007	25106	40	20200203*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 300 spectra of 7 reference samples from the substance/substance group *Calcium gluconate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 662 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 410 spectra of 12 reference samples from the substance/substance group *Calcium gluconate*.

- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Calcium gluconate	154356	23360	40
Caelo	Calcium gluconate	181010	24017	40
Caelo	Calcium gluconate	190240	24566	40
Caelo	Calcium gluconate	20004137011	25986	40
Caelo	Calcium gluconate	22001257	26250	40
Caelo	Calcium gluconate	24000791	27223	40
Euro OTC	Calcium gluconate	1606034	22699	40
Euro OTC	Calcium gluconate	1905015	24791	40
Fagron	Calcium gluconate	22D13-B03-229458	26666	40
Caelo	Calcium gluconate	20004137011	25986SI	10
Caelo	Calcium gluconate	22001257	26250SI	20
Fagron	Calcium gluconate	22D13-B03-229458	26666SI	20

- 201 674 spectra from a total of 4036 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 278 spectra from 160 *Apo-Ident* customers from 85 batches from the substance/substance group *Calcium gluconate*.

- Among them are spectra of independent samples from 82 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Calcium gluconate	171200-02	1
	Calcium gluconate	21003557009	1
	Calcium gluconate	22001257006	4
	Calcium gluconate	22001257008	1
AHD	Calcium gluconate	1911017-03	1
AHD	Calcium gluconate	21003557007	1
AHD	Calcium gluconate	22001257003	5
apomix	Calcium gluconate	1905015-02	1
Berkel AHK	Calcium gluconate	14085407	2
Caelo	Calcium gluconate	1000041-01	1
Caelo	Calcium gluconate	12335810	1
Caelo	Calcium gluconate	12335813	1
Caelo	Calcium gluconate	1407041-01	1
Caelo	Calcium gluconate	140704102	1
Caelo	Calcium gluconate	1407041-02	3
Caelo	Calcium gluconate	14085405	1
Caelo	Calcium gluconate	14230706	1
Caelo	Calcium gluconate	15126301	1
Caelo	Calcium gluconate	15324806	1
Caelo	Calcium gluconate	15324807	1
Caelo	Calcium gluconate	15435601	2
Caelo	Calcium gluconate	15435607	2
Caelo	Calcium gluconate	15435610	1
Caelo	Calcium gluconate	15435611	1
Caelo	Calcium gluconate	15435613	1
Caelo	Calcium gluconate	15435619	4
Caelo	Calcium gluconate	15435620	2
Caelo	Calcium gluconate	15435622	2
Caelo	Calcium gluconate	1543601	1
Caelo	Calcium gluconate	1606034	1
Caelo	Calcium gluconate	1606034-01	1
Caelo	Calcium gluconate	16603401	1
Caelo	Calcium gluconate	171200-01	1
Caelo	Calcium gluconate	1712007_02	1
Caelo	Calcium gluconate	1712007-02	1
Caelo	Calcium gluconate	18101003	2
Caelo	Calcium gluconate	18101004	3
Caelo	Calcium gluconate	18101006	2
Caelo	Calcium gluconate	18101010	2
Caelo	Calcium gluconate	18106202	2
Caelo	Calcium gluconate	1900240002	1
Caelo	Calcium gluconate	190240001	2
Caelo	Calcium gluconate	190240002	10
Caelo	Calcium gluconate	19024006	5
Caelo	Calcium gluconate	19024009	2
Caelo	Calcium gluconate	190240096	1
Caelo	Calcium gluconate	1905015-01	1
Caelo	Calcium gluconate	190772007	1
Caelo	Calcium gluconate	19240002	1
Caelo	Calcium gluconate	20004137002	5
Caelo	Calcium gluconate	20004137004	1
Caelo	Calcium gluconate	20004137006	3
Caelo	Calcium gluconate	21003557007	2
Caelo	Calcium gluconate	22001257003	1
Caelo	Calcium gluconate	4(18101004)	1
Caesar & Loretz GmbH...	Calcium gluconate	20004137006	2
Caesar & Loretz GmbH	Calcium gluconate	19024006	2
Caesar & Loretz GmbH	Calcium gluconate	19024009	1
Caesar & Loretz GmbH	Calcium gluconate	20004137002	2
Caesar & Loretz GmbH	Calcium gluconate	20004137005	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Calcium gluconate	20004137006	1
Caesar & Loretz GmbH	Calcium gluconate	20004137011	2
Caesar & Loretz GmbH	Calcium gluconate	21003557007	1
Caesar & Loretz GmbH	Calcium gluconate	22001257002	2
Caesar&Lorenz/AHD	Calcium gluconate	19024009	1
Caleo/ Noweda	Calcium gluconate	18101004	2
Eurho/Sns	Calcium gluconate	1209006-01	1
EuRho	Calcium gluconate	12090006-01	1
EuRho	Calcium gluconate	1209006-01	2
EuRho	Calcium gluconate	1304012-01	1
Euro OTC	Calcium gluconate	1105027-01	1
Euro OTC	Calcium gluconate	1105027-02	3
Euro OTC	Calcium gluconate	115027-01	1
Euro OTC	Calcium gluconate	1209006-01	7
Euro OTC	Calcium gluconate	1210001287	1
Euro OTC	Calcium gluconate	1304012-01	6
Euro OTC	Calcium gluconate	130401202	1
Euro OTC	Calcium gluconate	1304012-02	2
Euro OTC	Calcium gluconate	140704101	1
Euro OTC	Calcium gluconate	1407041-01	6
Euro OTC	Calcium gluconate	140704102	1
Euro OTC	Calcium gluconate	1407041-02	7
Euro OTC	Calcium gluconate	1602001644	3
Euro OTC	Calcium gluconate	1606034-01	20
Euro OTC	Calcium gluconate	1606034-02	10
Euro OTC	Calcium gluconate	1702000290	1
Euro OTC	Calcium gluconate	1712007	1
Euro OTC	Calcium gluconate	1712007-01	11
Euro OTC	Calcium gluconate	1712007-02	11
Euro OTC	Calcium gluconate	1712007-03	1
Euro OTC	Calcium gluconate	1712007-04	11
Euro OTC	Calcium gluconate	1905015-01	16
Euro OTC	Calcium gluconate	1905015-02	11
Euro OTC	Calcium gluconate	1911017-01	1
Euro OTC	Calcium gluconate	20270912-1	1
Euro OTC	Calcium gluconate	513-Q1211	1
Euro/Gehe	Calcium gluconate	1304012-01	1
Fagron	Calcium gluconate	10G22-N12	1
Fagron	Calcium gluconate	12D17-N01	1
Fagron	Calcium gluconate	14D11-B04	1
Fagron	Calcium gluconate	14D11-B04-294136	2
Fagron	Calcium gluconate	15D13-B98-307445	1
Fagron	Calcium gluconate	17E30-B02-343011	1
Finze	Calcium gluconate	917857359	1
Gatt-Koller / Phoenix	Calcium gluconate	550/03141214	1
Gehe/EuRo	Calcium gluconate	1712007-01	1
GEHE	Calcium gluconate	15435619	1
Gehe	Calcium gluconate	20004137011	1
L12	Calcium gluconate	15435627	1
Noweda	Calcium gluconate	15435627	1
Pharmachem	Calcium gluconate	18101003	1
Phönix/Euro	Calcium gluconate	1606034-01	1
Phönix	Calcium gluconate	1606034-01	1
sanacorp	Calcium gluconate	1407041-01	1
Sidonia	Calcium gluconate	18101004	1

- 235 789 spectra from 1515 *Apo-Ident* customers from a total of 49 174 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Calcium gluconate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Calcium gluconate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	410	0	201 674
Type C	0	278	0	235 789

The substance/substance group *Calcium gluconate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.5366 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 97.8417 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20871	20871	0.00	151.25
21283	21283	0.00	143.28
21312	20871	11.02	151.89
21821	23873	3.80	142.14
23873	23873	0.00	141.97
25086	25086	0.00	155.09
25106	25106	0.00	144.98

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Calcium glycerophosphate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20352-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Calcium glycerophosphate; Calcii glycerophosphas

Special notes

When selecting the *Calcium glycerophosphate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Calcium glycerophosphate	7	4	70

Second-stage model

For differentiation of the substance/substance group *Calcium glycerophosphate* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Calcium glycerophosphate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	45.29	–
Polymyxin B sulfate	46.82	17.33
⋮	⋮	⋮
Selenium yeast	>50	20.18
Amphotericin B	>50	23.03
Colistin sulfate	>50	23.22
Bacitracin	>50	34.79
SyrSpend® SF pH4 neo (Maize starch)	>50	38.60
Calcium pantothenate	>50	39.23
Riboflavin	>50	46.49
Nystatin	>50	48.88
SyrSpend® SF Alka	>50	57.09
Carmellose sodium	>50	62.59
Rice starch	>50	66.91
Cyanocobalamin	>50	71.40
Tosylchloramide sodium	>50	78.65
Gelatine, white	>50	80.06
SyrSpend® SF pH4	>50	81.00
Estradiol hemihydrate	>50	83.46
alpha-tocopheryl acetate dry concentrate	>50	85.43
Hyoscine hydrobromide	>50	88.65
Triamcinolone	>50	90.69
Methylcobalamin	>50	93.98
Acacia, dried dispersion	>50	94.65
Corn starch	>50	94.71
Wheat starch	>50	105.39
Oxalic acid	>50	115.96
Potato starch	>50	120.87
Estriol	>50	130.27
Maltodextrin	>50	134.48
Fructose	>50	155.17

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Calcium glycerophosphate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Calcium glycerophosphate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Calcium glycerophosphate	13007912	21311	40	20130124
Caelo	Calcium glycerophosphate	14341007	21969	60	AR-16-FG-005932-01
Caelo	Calcium glycerophosphate	191007	24538	40	20190502*
Caelo	Calcium glycerophosphate	20000551	25228	40	20200708*
Caelo	Calcium glycerophosphate	21000588	25634	40	20210217*
Fagron	Calcium glycerophosphate	13I17-N04	21234	40	20131016
Fagron	Calcium glycerophosphate	15B03-B03-305050	21978	60	1706313

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 320 spectra of 7 reference samples from the substance/substance group *Calcium glycerophosphate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.
- 152 642 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 170 spectra of 5 reference samples from the substance/substance group *Calcium glycerophosphate*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Calcium glycerophosphate	12012411	20679	40
Caelo	Calcium glycerophosphate	12012417	20771	40
Caelo	Calcium glycerophosphate	162310	23361	40
Caelo	Calcium glycerophosphate	20004507	26309	30
Caelo	Calcium glycerophosphate	20004507	26309SI	20

- 201 914 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 214 spectra from 127 *Apo-Ident* customers from 73 batches from the substance/substance group *Calcium glycerophosphate*.

- Among them are spectra of independent samples from 70 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Calcium glycerophosphate	B03-2224201	1
AHD	Calcium glycerophosphate	20004507016	1
AHD	Calcium glycerophosphate	20004507017	2
Caelo	Calcium glycerophosphate	12012406	1
Caelo	Calcium glycerophosphate	12012413	2
Caelo	Calcium glycerophosphate	13007902	1
Caelo	Calcium glycerophosphate	13007908	1
Caelo	Calcium glycerophosphate	13007912	2
Caelo	Calcium glycerophosphate	13007914	1
Caelo	Calcium glycerophosphate	13A18-N02	2
Caelo	Calcium glycerophosphate	13A18-No2	1
Caelo	Calcium glycerophosphate	14341007	5
Caelo	Calcium glycerophosphate	14341009	1
Caelo	Calcium glycerophosphate	14341010	1
Caelo	Calcium glycerophosphate	14341013	1
Caelo	Calcium glycerophosphate	14341015	1
Caelo	Calcium glycerophosphate	14347101	2
Caelo	Calcium glycerophosphate	14B10-B02-296841	1
Caelo	Calcium glycerophosphate	15B03B03305050	1
Caelo	Calcium glycerophosphate	15B03-B03-305050	1
Caelo	Calcium glycerophosphate	162310	1
Caelo	Calcium glycerophosphate	16231001	3
Caelo	Calcium glycerophosphate	16231004	3
Caelo	Calcium glycerophosphate	16231005	1
Caelo	Calcium glycerophosphate	16231006	4
Caelo	Calcium glycerophosphate	16231007	2
Caelo	Calcium glycerophosphate	16231008	2
Caelo	Calcium glycerophosphate	16231010	5
Caelo	Calcium glycerophosphate	17250703	5
Caelo	Calcium glycerophosphate	17359101	14
Caelo	Calcium glycerophosphate	17359101P-180122-1	1
Caelo	Calcium glycerophosphate	17359106	8
Caelo	Calcium glycerophosphate	17359107	9
Caelo	Calcium glycerophosphate	17359107P-181218-2	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Calcium glycerophosphate	17359110	1
Caelo	Calcium glycerophosphate	17359111	1
Caelo	Calcium glycerophosphate	180918A	1
Caelo	Calcium glycerophosphate	190762007	1
Caelo	Calcium glycerophosphate	191007001	3
Caelo	Calcium glycerophosphate	19100701	1
Caelo	Calcium glycerophosphate	19100702	5
Caelo	Calcium glycerophosphate	19100703	18
Caelo	Calcium glycerophosphate	19100707	5
Caelo	Calcium glycerophosphate	20000551002	1
Caelo	Calcium glycerophosphate	20000551003	4
Caelo	Calcium glycerophosphate	20004507001	2
Caelo	Calcium glycerophosphate	20004507004	3
Caelo	Calcium glycerophosphate	20004507005	1
Caelo	Calcium glycerophosphate	20004507007	2
Caelo	Calcium glycerophosphate	20004507014	2
Caelo	Calcium glycerophosphate	20004507016	2
Caelo	Calcium glycerophosphate	2004507001	1
Caelo	Calcium glycerophosphate	2004507017	1
Caesar & Loretz GmbH...	Calcium glycerophosphate	20004507017	1
Caesar & Loretz GmbH...	Calcium glycerophosphate	21000588001	2
Caesar & Loretz GmbH...	Calcium glycerophosphate	20004507001	2
Caesar & Loretz GmbH	Calcium glycerophosphate	191007001	2
Caesar & Loretz GmbH	Calcium glycerophosphate	19100703	1
Caesar & Loretz GmbH	Calcium glycerophosphate	19100707	1
Caesar & Loretz GmbH	Calcium glycerophosphate	20000551003	2
Caesar & Loretz GmbH	Calcium glycerophosphate	20004507001	2
Caesar & Loretz GmbH	Calcium glycerophosphate	20004507004	3
Caesar & Loretz GmbH	Calcium glycerophosphate	20004507007	3
Caesar & Loretz GmbH	Calcium glycerophosphate	20004507014	2
Caesar&Lorenz/AHD	Calcium glycerophosphate	16231010	1
Cealo/Sanacorp	Calcium glycerophosphate	17359101	1
Fagron	Calcium glycerophosphate	11G19-N05	1
Fagron	Calcium glycerophosphate	1216000005	1
Fagron	Calcium glycerophosphate	12I18-N06	3
Fagron	Calcium glycerophosphate	1314000019	1
Fagron	Calcium glycerophosphate	1317-N04	2
Fagron	Calcium glycerophosphate	13A18N02	2
Fagron	Calcium glycerophosphate	13A18-N02	5
Fagron	Calcium glycerophosphate	14B10B02	1
Fagron	Calcium glycerophosphate	14B10-B02	1
Fagron	Calcium glycerophosphate	14B10-B02-291642	1
Fagron	Calcium glycerophosphate	14B10-B02-296841	4
Fagron	Calcium glycerophosphate	15B03B03	1
Fagron	Calcium glycerophosphate	15B03-B03	1
Fagron	Calcium glycerophosphate	15B03-B03-305050	3
Fagron	Calcium glycerophosphate	17J17-B07-3583	1
Fagron	Calcium glycerophosphate	19J10-F06-366452	3
Fagron	Calcium glycerophosphate	2417Q-01212	1
Fagron	Calcium glycerophosphate	3115A-01212	1
Fagron	Calcium glycerophosphate	5212M-01212	1
Fagron	Calcium glycerophosphate	700338-0002	1
Gatt-Koller/Kwizda	Calcium glycerophosphate	4007/09123812	1
Gehe	Calcium glycerophosphate	16231006	1
Gehe	Calcium glycerophosphate	17359108	1
Gehe	Calcium glycerophosphate	19100701	2
Gehe	Calcium glycerophosphate	19100703	1
Gehe	Calcium glycerophosphate	20004507016	1
Phönix	Calcium glycerophosphate	20004507004	1
Sanacorp	Calcium glycerophosphate	16231008	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Calcium glycerophosphate	17359102	1
Sanacorp	Calcium glycerophosphate	20000551002	1
Sanacorp	Calcium glycerophosphate	20004507007	1
Sidonia	Calcium glycerophosphate	17250703	1

- 235 853 spectra from 1515 *Apo-Ident* customers from a total of 49 186 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Calcium glycerophosphate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Calcium glycerophosphate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	170	0	201 914
Type C	0	214	0	235 853

The substance/substance group *Calcium glycerophosphate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.4706 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 97.1963 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21234	21969	14.87	50.95
21311	21969	9.53	49.70

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21969	21969	0.00	50.81
21978	21978	0.00	46.94
24538	24538	0.00	46.85
25228	25228	0.00	42.94
25634	25634	0.00	44.94

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Calcium hydrogen phosphate dihydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20129-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Calcium hydrogen phosphate dihydrate; Calcii hydrogenphosphas dihydricus

Special notes

When selecting the *Calcium hydrogen phosphate dihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Calcium hydrogen phosphate dihydrate	2	1	21

Second-stage model

For differentiation of the substance/substance group *Calcium hydrogen phosphate dihydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Calcium hydrogen phosphate dihydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	58.83	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Calcium hydrogen phosphate dihydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Calcium hydrogen phosphate dihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Calcium hydrogen phosphat…	181117	24225	40	20180528*
Caelo	Calcium hydrogen phosphat…	22001222	26566	40	20220607*
Caelo	Calcium hydrogen phosphat…	22001222	26566SI	20	20220607*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 100 spectra of 3 reference samples from the substance/substance group *Calcium hydrogen phosphate dihydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 862 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 60 spectra of 2 reference samples from the substance/substance group *Calcium hydrogen phosphate dihydrate*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Calcium hydrogen phosphat…	23002987	27080	40
Caelo	Calcium hydrogen phosphat…	23002987	27080SI	20

- 202 024 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 38 spectra from 26 *Apo-Ident* customers from 21 batches from the substance/substance group *Calcium hydrogen phosphate dihydrate*.

- Among them are spectra of independent samples from 21 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Calcium hydrogen phosphat…	101352009	1
Caelo	Calcium hydrogen phosphat…	10135201	1
Caelo	Calcium hydrogen phosphat…	10135216	1
Caelo	Calcium hydrogen phosphat…	10135223	1
Caelo	Calcium hydrogen phosphat…	10135228	1
Caelo	Calcium hydrogen phosphat…	11287501	1
Caelo	Calcium hydrogen phosphat…	11287503	2
Caelo	Calcium hydrogen phosphat…	11287509	2
Caelo	Calcium hydrogen phosphat…	11287510	1
Caelo	Calcium hydrogen phosphat…	12212804	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Calcium hydrogen phosphat…	12212806	1
Caelo	Calcium hydrogen phosphat…	12212807	1
Caelo	Calcium hydrogen phosphat…	12212811	4
Caelo	Calcium hydrogen phosphat…	12212812	2
Caelo	Calcium hydrogen phosphat…	12212813	1
Caelo	Calcium hydrogen phosphat…	12212816	1
Caelo	Calcium hydrogen phosphat…	12212822	1
Caelo	Calcium hydrogen phosphat…	13170701	6
Caelo	Calcium hydrogen phosphat…	13170704	1
Caelo	Calcium hydrogen phosphat…	14011401	1
Caelo	Calcium hydrogen phosphat…	14085301	1
Cealo	Calcium hydrogen phosphat…	12212811	1
Phönix 12.12.2013	Calcium hydrogen phosphat…	13170704	1

- 236 029 spectra from 1515 *Apo-Ident* customers from a total of 49 237 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Calcium hydrogen phosphate dihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Calcium hydrogen phosphate dihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	100	0	152 862
Type B	0	60	0	202 024
Type C	0	33	5	236 029

The substance/substance group *Calcium hydrogen phosphate dihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.9007 %)	86.8421 % (> 78.9474 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24225	24225	0.00	107.87
26566	26566	0.00	107.25

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Calcium lactate pentahydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20745-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Calcium lactate pentahydrate; Calcii lactas pentahydricus

Special notes

When selecting the *Calcium lactate pentahydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Calcium lactate pentahydrate	7	5	46

Second-stage model

For differentiation of the substance/substance group *Calcium lactate pentahydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Calcium lactate pentahydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	48.93	–
Riboflavin sodium phosphate hydrate	53.06	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Calcium lactate pentahydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Calcium lactate pentahydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Calcium lactate pentahydrate	15101401	21909	60	20150407
Caelo	Calcium lactate pentahydrate	15101405	22263	60	20150407
Caelo	Calcium lactate pentahydrate	161313	22445	60	20160513*
Caelo	Calcium lactate pentahydrate	20000512	25225	40	20200320*
Caelo	Calcium lactate pentahydrate	23002025	26971	40	20230918*
Caelo	Calcium lactate pentahydrate	23002025	26971SI	20	20230918*
Fagron	Calcium lactate pentahydrate	12E10-N03	20745	40	20120704
Fagron	Calcium lactate pentahydrate	12I12-N06	21232	40	AR-15-FG-007939-01

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 8 reference samples from the substance/substance group *Calcium lactate pentahydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 602 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Calcium lactate pentahydrate*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Calcium lactate pentahydrate	171377	23642	40
Caelo	Calcium lactate pentahydrate	180734	24035	40
Caelo	Calcium lactate pentahydrate	24002487	27428	40
Fagron	Calcium lactate pentahydrate	14H01-B05-323830	23566	40
Fagron	Calcium lactate pentahydrate	23C16-B11-234646	27036	40
Caelo	Calcium lactate pentahydrate	24002487	27428SI	20
Fagron	Calcium lactate pentahydrate	23C16-B11-234646	27036SI	20

- 201 844 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 79 spectra from 38 *Apo-Ident* customers from 48 batches from the substance/substance group *Calcium lactate pentahydrate*.

- Among them are spectra of independent samples from 46 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Calcium lactate pentahydrate	11369606	1
Caelo	Calcium lactate pentahydrate	11369610	1
Caelo	Calcium lactate pentahydrate	11369614	2
Caelo	Calcium lactate pentahydrate	11369618	1
Caelo	Calcium lactate pentahydrate	12C15-N02	1
Caelo	Calcium lactate pentahydrate	12E10-N03	1
Caelo	Calcium lactate pentahydrate	13080802	2
Caelo	Calcium lactate pentahydrate	13080804	2
Caelo	Calcium lactate pentahydrate	13080805	2
Caelo	Calcium lactate pentahydrate	14H01B05300502	1
Caelo	Calcium lactate pentahydrate	15101409	1
Caelo	Calcium lactate pentahydrate	15101411	2
Caelo	Calcium lactate pentahydrate	15101412	3
Caelo	Calcium lactate pentahydrate	15227804	2
Caelo	Calcium lactate pentahydrate	16131302	1
Caelo	Calcium lactate pentahydrate	16131307	1
Caelo	Calcium lactate pentahydrate	16131312	1
Caelo	Calcium lactate pentahydrate	16333106	4
Caelo	Calcium lactate pentahydrate	16333111	4
Caelo	Calcium lactate pentahydrate	16333113	1
Caelo	Calcium lactate pentahydrate	17137707	2
Caelo	Calcium lactate pentahydrate	17355503	2
Caelo	Calcium lactate pentahydrate	17J18-B01-350892	1
Caelo	Calcium lactate pentahydrate	18073406	2
Caelo	Calcium lactate pentahydrate	18073413	2
Caelo	Calcium lactate pentahydrate	18073415	2
Caelo	Calcium lactate pentahydrate	19042203	2
Caelo	Calcium lactate pentahydrate	19042208	1
Caelo	Calcium lactate pentahydrate	20000512004	1
Caelo	Calcium lactate pentahydrate	20003749002	1
Caelo	Calcium lactate pentahydrate	20003749008	1
Fagron	Calcium lactate pentahydrate	12/12-N06	1
Fagron	Calcium lactate pentahydrate	12C15-N02	1
Fagron	Calcium lactate pentahydrate	12I12-N01	1
Fagron	Calcium lactate pentahydrate	12I12-N06	2
Fagron	Calcium lactate pentahydrate	13L18B04	1
Fagron	Calcium lactate pentahydrate	13L18-B04-295541	3
Fagron	Calcium lactate pentahydrate	14H01-B05	1
Fagron	Calcium lactate pentahydrate	14H01-B05-334588	2
Fagron	Calcium lactate pentahydrate	17J18-B01-343387	1
Fagron	Calcium lactate pentahydrate	17J18-B01-347174	1
Fagron	Calcium lactate pentahydrate	1806000537	1
Fagron	Calcium lactate pentahydrate	1901001645	1
Fagron	Calcium lactate pentahydrate	19B26-B05	1
Fagron	Calcium lactate pentahydrate	20C31-B02-201355	2
Fagron	Calcium lactate pentahydrate	21B23-B02-210092	2
Fagron	Calcium lactate pentahydrate	21B23-BO2-210092	1
Fagron	Calcium lactate pentahydrate	21F09-B02-215877	3
Phönix	Calcium lactate pentahydrate	14H01-B05	1
phönix	Calcium lactate pentahydrate	15101411	1
Shop	Calcium lactate pentahydrate	1111001829	1

- 235 988 spectra from 1515 *Apo-Ident* customers from a total of 49 210 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Calcium lactate pentahydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Calcium lactate pentahydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	240	0	201 844
Type C	0	79	0	235 988

The substance/substance group *Calcium lactate pentahydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 92.4051 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20745	22445	7.66	139.53
21232	21232	0.00	136.66
21909	22445	8.28	141.22
22263	22445	6.68	139.14
22445	22445	0.00	141.91
25225	25225	0.00	137.58
26971	26971	0.00	144.12

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Calcium pantothenate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20395-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Calcium pantothenate; Calcii pantothenas

Special notes

When selecting the *Calcium pantothenate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Calcium pantothenate	11	10	78

Second-stage model

For differentiation of the substance/substance group *Calcium pantothenate* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Calcium pantothenate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	18.40	13.04
Colistin sulfate	53.28	16.07
⋮	⋮	⋮
Bacitracin	59.49	15.49
Methylcobalamin	>50	34.15
Amphotericin B	>50	41.16
Cyanocobalamin	>50	52.64
Nystatin	>50	56.76
Gelatine, white	>50	58.17
Riboflavin	>50	61.84
Triamcinolone	>50	67.61
Estradiol hemihydrate	>50	78.19
alpha-tocopheryl acetate dry concentrate	>50	82.21
Selenium yeast	>50	87.36
Calcium glycerophosphate	>50	95.43
Estriol	>50	108.61
Carmellose sodium	>50	128.33
Hyoscine hydrobromide	>50	129.34
SyrSpend® SF Alka	>50	156.90
Tosylchloramide sodium	>50	163.34
Rice starch	>50	192.84
SyrSpend® SF pH4 neo (Maize starch)	>50	227.36
Oxalic acid	>50	249.76
Acacia, dried dispersion	>50	261.69
Corn starch	>50	281.12
SyrSpend® SF pH4	>50	307.09
Potato starch	>50	383.72
Maltodextrin	>50	388.25
Wheat starch	>50	389.13
Fructose	>50	407.10

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Calcium pantothenate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Calcium pantothenate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Calcium pantothenate	14208012	21765	60	20140722
Caelo	Calcium pantothenate	173352	24045	40	20180202*
Euro OTC	Calcium pantothenate	1305034-01	21243	40	20130617
Euro OTC	Calcium pantothenate	1509024	21901	60	20151005*
Euro OTC	Calcium pantothenate	1603042	22551	40	20160429*
Euro OTC	Calcium pantothenate	1607023	22691	40	20160809*
Euro OTC	Calcium pantothenate	1702018	23153	40	20170330*
Euro OTC	Calcium pantothenate	1711003	23890	40	20171123*
Euro OTC	Calcium pantothenate	2008019	25296	40	20200921*
Euro OTC	Calcium pantothenate	2101037	25592	40	20210304*
Fagron	Calcium pantothenate	13H28-N11	21233	40	20130916

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 480 spectra of 11 reference samples from the substance/substance group *Calcium pantothenate*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.
- 152 482 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 450 spectra of 13 reference samples from the substance/substance group *Calcium pantothenate*.
- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Calcium pantothenate	162516	23363	40
Caelo	Calcium pantothenate	15344217	23717	40
Caelo	Calcium pantothenate	21003241008	26303	30
Caelo	Calcium pantothenate	23000511	26724	40
Euro OTC	Calcium pantothenate	1803014	24081	40
Euro OTC	Calcium pantothenate	1809014	24312	40
Euro OTC	Calcium pantothenate	1902032	24479	40
Euro OTC	Calcium pantothenate	2003007	25241	40
Euro OTC	Calcium pantothenate	2111014	25873	50
Euro OTC	Calcium pantothenate	2311018	27070	40
Caelo	Calcium pantothenate	21003241008	26303SI	20
Caelo	Calcium pantothenate	23000511	26724SI	20
Euro OTC	Calcium pantothenate	2111014	25873SI	10

- 201 634 spectra from a total of 4035 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 198 spectra from 85 *Apo-Ident* customers from 82 batches from the substance/substance group *Calcium pantothenate*.

- Among them are spectra of independent samples from 78 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Calcium pantothenate	21003241015	1
	Calcium pantothenate	2111014-01	1
	Calcium pantothenate	22002458007	1
	Calcium pantothenate	23000511	1
	Calcium pantothenate	2301036-01	2
AHD	Calcium pantothenate	15344221	1
Anzag/Anzag 26.07.18	Calcium pantothenate	1803017-01	1
Caelo	Calcium pantothenate		1
Caelo	Calcium pantothenate	1013Q-03022	1
Caelo	Calcium pantothenate	11105731	1
Caelo	Calcium pantothenate	12236622	1
Caelo	Calcium pantothenate	12340808	3
Caelo	Calcium pantothenate	12340809	1
Caelo	Calcium pantothenate	12340819	2
Caelo	Calcium pantothenate	12340832	1
Caelo	Calcium pantothenate	12340846	1
Caelo	Calcium pantothenate	12340859	1
Caelo	Calcium pantothenate	1410011-01	1
Caelo	Calcium pantothenate	1410011-02	1
Caelo	Calcium pantothenate	14208004	1
Caelo	Calcium pantothenate	1509024-01	1
Caelo	Calcium pantothenate	15344207	1
Caelo	Calcium pantothenate	15344214	1
Caelo	Calcium pantothenate	1603042-01	1
Caelo	Calcium pantothenate	16251608	2
Caelo	Calcium pantothenate	1711003-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Calcium pantothenate	17335208	5
Caelo	Calcium pantothenate	17335209	1
Caelo	Calcium pantothenate	18174608	1
Caelo	Calcium pantothenate	19057402	1
Caelo	Calcium pantothenate	19067402	2
Caelo	Calcium pantothenate	19067404	1
Caelo	Calcium pantothenate	19067405	2
Caelo	Calcium pantothenate	190751002	5
Caelo	Calcium pantothenate	190751004	3
Caelo	Calcium pantothenate	192718003	3
Caelo	Calcium pantothenate	192718004	5
Caelo	Calcium pantothenate	20004234001	3
Caelo	Calcium pantothenate	20004234003	1
Caelo	Calcium pantothenate	20004252009	1
Caelo	Calcium pantothenate	21003241008	2
Caelo	Calcium pantothenate	27111303	1
Caelo	Calcium pantothenate	8041407	1
Caesar & Loretz GmbH...	Calcium pantothenate	20004252012	1
Caesar & Loretz GmbH...	Calcium pantothenate	21003241008	3
Caesar & Loretz GmbH...	Calcium pantothenate	19067404	1
Caesar & Loretz GmbH/Phoe	Calcium pantothenate	20004234001	2
Caesar & Loretz GmbH...	Calcium pantothenate	190751002	1
Caesar & Loretz GmbH...	Calcium pantothenate	192718004	1
Caesar & Loretz GmbH	Calcium pantothenate	17335209	2
Caesar & Loretz GmbH	Calcium pantothenate	19067404	1
Caesar & Loretz GmbH	Calcium pantothenate	190751002	5
Caesar & Loretz GmbH	Calcium pantothenate	192718003	1
Caesar & Loretz GmbH	Calcium pantothenate	192718004	2
Caesar & Loretz GmbH	Calcium pantothenate	20004252009	2
Caesar/Gehe	Calcium pantothenate	17335209	2
EuRho/sanacorp	Calcium pantothenate	1803014-01	1
Euro OTC	Calcium pantothenate	10021505	1
Euro OTC	Calcium pantothenate	1111025-01	1
Euro OTC	Calcium pantothenate	1209022-01	1
Euro OTC	Calcium pantothenate	1209022-02	1
Euro OTC	Calcium pantothenate	1209022-02pzn	1
Euro OTC	Calcium pantothenate	130503401	2
Euro OTC	Calcium pantothenate	1305034-01	4
Euro OTC	Calcium pantothenate	1312027-01	3
Euro OTC	Calcium pantothenate	1410011-01	1
Euro OTC	Calcium pantothenate	1410011-02	3
Euro OTC	Calcium pantothenate	1509024-01	3
Euro OTC	Calcium pantothenate	1603042-01	4
Euro OTC	Calcium pantothenate	1607023-01	5
Euro OTC	Calcium pantothenate	1702018-01	3
Euro OTC	Calcium pantothenate	17021401	1
Euro OTC	Calcium pantothenate	1711003-01	7
Euro OTC	Calcium pantothenate	1803014-01	4
Euro OTC	Calcium pantothenate	1809014-01	2
Euro OTC	Calcium pantothenate	18111707	1
Euro OTC	Calcium pantothenate	1902023-01	1
Euro OTC	Calcium pantothenate	190203201	1
Euro OTC	Calcium pantothenate	1902032-01	2
Euro OTC	Calcium pantothenate	190203202	1
Euro OTC	Calcium pantothenate	1902032-02	4
Euro OTC	Calcium pantothenate	2001037-01	1
Euro OTC	Calcium pantothenate	200300701	1
Euro OTC	Calcium pantothenate	2003007-01	6
Euro OTC	Calcium pantothenate	2008019-01	6
Euro OTC	Calcium pantothenate	201037-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Calcium pantothenate	2101037-01	6
Euro OTC	Calcium pantothenate	2111014-01	7
Euro OTC	Calcium pantothenate	2111014-02	1
Euro OTC	Calcium pantothenate	2301036-01	1
Euro OTC	Calcium pantothenate	5121405	1
Euro OTC	Calcium pantothenate	99142536W0	1
Euroo/Anzag	Calcium pantothenate	1509024-01	2
Fagron	Calcium pantothenate	1111025-01	1
Fagron	Calcium pantothenate	1111110405	1
Fagron	Calcium pantothenate	12F19-N07	1
Fagron	Calcium pantothenate	13H28-N11	1
Fagron	Calcium pantothenate	14G02-B10-297373	1
Gehe Pharma Handel	Calcium pantothenate	22002458006	1
Gehe	Calcium pantothenate	1004024-01	1
Hangzhou xinfu	Calcium pantothenate	2008019-01	2
Nachprüfung	Calcium pantothenate	123456	1
Noweda	Calcium pantothenate	14208012	1
Noweda	Calcium pantothenate	TL017107823	1
Sanacorp	Calcium pantothenate	17335203	1

- 235 869 spectra from 1515 *Apo-Ident* customers from a total of 49 179 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Calcium pantothenate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Calcium pantothenate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	480	0	152 482
Type B	0	450	0	201 634
Type C	0	198	0	235 869

The substance/substance group *Calcium pantothenate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6667 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 96.9697 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21233	23890	20.37	60.33
21243	24045	15.83	58.25
21765	24045	11.55	58.25
21901	21901	0.00	59.49
22551	22551	0.00	36.93
22691	22691	0.00	41.68
23153	23153	0.00	59.36
23890	23890	0.00	59.68
24045	24045	0.00	58.45
25296	25296	0.00	63.36
25592	25592	0.00	49.51

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Camphor, racemic/D-Camphor**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	25048-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Camphor, racemic/D-Camphor; Camphor, racemic; Camphora racemica; D-Camphor; D-Camphora

Special notes

When selecting the *Camphor, racemic/D-Camphor* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Camphor, racemic/D-Camphor	10	11	81

Second-stage model

For differentiation of the substance/substance group *Camphor, racemic/D-Camphor* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Camphor, racemic/D-Camphor* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Spironolactone	76.52	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Camphor, racemic/D-Camphor* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Camphor, racemic/D-Camphor*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Camphor, racemic	15316801	25049	60	20151029
Caelo	Camphor, racemic	170043	25051	40	20170220*
Caelo	Camphor, racemic	192762	25562	40	20200127*
Caelo	Camphor, racemic	21002072014	25977	40	20210817
Euro OTC	Camphor, racemic	1406029-01	25048	60	20140708
Fagron	Camphor, racemic	14E19-B07-300365	25050	60	20140527
Fagron	Camphor, racemic	16E23-B08-336937	25053	40	20160627
Caelo	D-Camphor	162354	24680	40	20160809*
Caelo	D-Camphor	23000933	27262	40	20230505*
Gatt-Koller	D-Camphor	23J02066	27091	40	20231109
Gatt-Koller	D-Camphor	23J02066	27091SI	20	20231109

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 480 spectra of 11 reference samples from the substance/substance group *Camphor, racemic/D-Camphor*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 482 spectra from a total of 2832 batches from further 482 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 500 spectra of 15 reference samples from the substance/substance group *Camphor, racemic/D-Camphor*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Camphor, racemic	183279	24728	40
Caelo	Camphor, racemic	192454	24876	40
Caelo	Camphor, racemic	16209309	25052	40
Caelo	Camphor, racemic	172883	25054	40
Caelo	Camphor, racemic	180198	25055	40
Caelo	Camphor, racemic	21003662	25994	40
Caelo	Camphor, racemic	23001930	26947	40
Caelo	Camphor, racemic	24001181	27259	40
Fagron	Camphor, racemic	21K27-B05-226181	26462	40
Gatt-Koller	Camphor, racemic	21J02080	26704	40
Caelo	D-Camphor	190097	24681	40
Caelo	Camphor, racemic	21002072014	25977SI†	10
Caelo	Camphor, racemic	21003662	25994SI	10
Fagron	Camphor, racemic	21K27-B05-226181	26462SI	20
Caelo	D-Camphor	23000933	27262SI†	20

- 201 584 spectra from a total of 4032 batches from further 837 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 362 spectra from 240 *Apo-Ident* customers from 82 batches from the substance/substance group *Camphor, racemic/D-Camphor*.
- Among them are spectra of independent samples from 81 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Camphor, racemic	16235408	1
	Camphor, racemic	21000070022	1
	Camphor, racemic	21003662006	2
	Camphor, racemic	21003662010	6
	Camphor, racemic	21003662011	1
	Camphor, racemic	22003278003	1
	Camphor, racemic	22003278004	3
	Camphor, racemic	22003278007	3
	Camphor, racemic	2203278007	1
	Camphor, racemic	24000108001	1
AHD	Camphor, racemic	192762005	1
Alliance Healthcare	Camphor, racemic	18196907	2
Alliance Healthcare	Camphor, racemic	22001161003	1
Caelo	Camphor, racemic	17004301	1
Caelo	Camphor, racemic	17050605	2
Caelo	Camphor, racemic	17288306	2
Caelo	Camphor, racemic	17288307	2
Caelo	Camphor, racemic	18019806	5
Caelo	Camphor, racemic	18066404	1
Caelo	Camphor, racemic	18108904	1
Caelo	Camphor, racemic	18196906	5
Caelo	Camphor, racemic	18196907	8
Caelo	Camphor, racemic	183279001	1
Caelo	Camphor, racemic	183279002	10
Caelo	Camphor, racemic	18327901	1
Caelo	Camphor, racemic	18327903	5
Caelo	Camphor, racemic	18327905	12
Caelo	Camphor, racemic	18327909	20
Caelo	Camphor, racemic	18327910	1
Caelo	Camphor, racemic	19009704	4
Caelo	Camphor, racemic	19245003	1
Caelo	Camphor, racemic	192454002	1
Caelo	Camphor, racemic	192454003	1
Caelo	Camphor, racemic	192454004	6
Caelo	Camphor, racemic	192454006	8
Caelo	Camphor, racemic	19262009	1
Caelo	Camphor, racemic	192762002	1
Caelo	Camphor, racemic	192762004	3
Caelo	Camphor, racemic	192762005	8
Caelo	Camphor, racemic	192762007	2
Caelo	Camphor, racemic	192762009	16
Caelo	Camphor, racemic	192823001	1
Caelo	Camphor, racemic	192823004	1
Caelo	Camphor, racemic	200003828001	1
Caelo	Camphor, racemic	20003828001	10
Caelo	Camphor, racemic	20003828002	3
Caelo	Camphor, racemic	20003828003	1
Caelo	Camphor, racemic	20003828006	3
Caelo	Camphor, racemic	20004261006	6
Caelo	Camphor, racemic	20004261007	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Camphor, racemic	21000070001	1
Caelo	Camphor, racemic	21000070003	1
Caelo	Camphor, racemic	21000070008	1
Caelo	Camphor, racemic	21000070011	1
Caelo	Camphor, racemic	21000070022	1
Caelo	Camphor, racemic	210020720009	1
Caelo	Camphor, racemic	21002072001	5
Caelo	Camphor, racemic	21002072002	8
Caelo	Camphor, racemic	21002072009	5
Caelo	Camphor, racemic	21002072013	1
Caelo	Camphor, racemic	21002072014	5
Caelo	Camphor, racemic	210020722002	1
Caelo	Camphor, racemic	21003662002	7
Caelo	Camphor, racemic	21003662003	1
Caelo	Camphor, racemic	21003662006	6
Caelo	Camphor, racemic	21003662010	2
Caelo	Camphor, racemic	2102072002	1
Caelo	Camphor, racemic	22003278007	1
Caelo	Camphor, racemic	5218Q-01221	1
Caelo	Camphor, racemic	63(192454004)	1
Caelo	Camphor, racemic	Caelo	1
Caelo	Camphor, racemic	Nachreichen	1
Caesar & Lorenz GmbH	Camphor, racemic	192762005	1
Caesar & Loretz GmbH…	Camphor, racemic	21002072002	1
Caesar & Loretz GmbH…	Camphor, racemic	18327901	1
Caesar & Loretz GmbH…	Camphor, racemic	21002072002	1
Caesar & Loretz GmbH…	Camphor, racemic	21002072014	1
Caesar & Loretz GmbH…	Camphor, racemic	21003662010	1
Caesar & Loretz GmbH/AHD	Camphor, racemic	21002072014	1
Caesar & Loretz GmbH…	Camphor, racemic	20003828001	1
Caesar & Loretz GmbH/Gehe	Camphor, racemic	183279	1
Caesar & Loretz GmbH/Now	Camphor, racemic	20003828001	1
Caesar & Loretz GmbH…	Camphor, racemic	183279002	1
Caesar & Loretz GmbH…	Camphor, racemic	18327905	1
Caesar & Loretz GmbH/Otto	Camphor, racemic	192762005	1
Caesar & Loretz GmbH…	Camphor, racemic	20004261007	1
Caesar & Loretz GmbH…	Camphor, racemic	192762007	1
Caesar & Loretz GmbH/Sa	Camphor, racemic	18327901	1
Caesar & Loretz GmbH…	Camphor, racemic	18327909	1
Caesar & Loretz GmbH…	Camphor, racemic	21003662010	1
Caesar & Loretz GmbH	Camphor, racemic	17288306	3
Caesar & Loretz GmbH	Camphor, racemic	18019807	1
Caesar & Loretz GmbH	Camphor, racemic	18019811	1
Caesar & Loretz GmbH	Camphor, racemic	18196906	2
Caesar & Loretz GmbH	Camphor, racemic	18196907	1
Caesar & Loretz GmbH	Camphor, racemic	183279002	2
Caesar & Loretz GmbH	Camphor, racemic	18327903	2
Caesar & Loretz GmbH	Camphor, racemic	18327905	3
Caesar & Loretz GmbH	Camphor, racemic	18327909	5
Caesar & Loretz GmbH	Camphor, racemic	18327910	4
Caesar & Loretz GmbH	Camphor, racemic	192454001	1
Caesar & Loretz GmbH	Camphor, racemic	192454004	7
Caesar & Loretz GmbH	Camphor, racemic	192454006	3
Caesar & Loretz GmbH	Camphor, racemic	192454007	1
Caesar & Loretz GmbH	Camphor, racemic	192762001	1
Caesar & Loretz GmbH	Camphor, racemic	192762005	2
Caesar & Loretz GmbH	Camphor, racemic	192762009	8
Caesar & Loretz GmbH	Camphor, racemic	20003828001	8
Caesar & Loretz GmbH	Camphor, racemic	20003828002	2
Caesar & Loretz GmbH	Camphor, racemic	20003828006	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Camphor, racemic	20004261002	1
Caesar & Loretz GmbH	Camphor, racemic	20004261005	1
Caesar & Loretz GmbH	Camphor, racemic	20004261006	1
Caesar & Loretz GmbH	Camphor, racemic	20004261007	2
Caesar & Loretz GmbH	Camphor, racemic	21002072001	2
Caesar & Loretz GmbH	Camphor, racemic	21002072002	3
Caesar & Loretz GmbH	Camphor, racemic	21002072009	4
Caesar & Loretz GmbH	Camphor, racemic	21002072012	1
Caesar & Loretz GmbH	Camphor, racemic	21002072013	1
Caesar & Loretz GmbH	Camphor, racemic	21002072014	3
Caesar & Loretz GmbH	Camphor, racemic	21003662002	3
Caesar & Loretz GmbH	Camphor, racemic	21003662003	1
Caesar & Loretz GmbH	Camphor, racemic	21003662006	3
Caesar&Loretz GmbH	Camphor, racemic	192454004	1
Caleo/Phoenix	Camphor, racemic	21002072009	1
campher racemischer	Camphor, racemic	21003662010	1
EuRho/Phönix	Camphor, racemic	21002072002	1
Euro OTC	Camphor, racemic	1202021	1
FIEBIG	Camphor, racemic	110-01	1
Gehe	Camphor, racemic	21003662010	1
Kehr	Camphor, racemic	21003662006	2
Klenk	Camphor, racemic	444A180815	5
Klenk	Camphor, racemic	444A200110-01	1
Noveda	Camphor, racemic	192762009	1
Noweda	Camphor, racemic	21002072014	1
Noweda	Camphor, racemic	22001161005	1
Oriental/Noweda	Camphor, racemic	102/1819	1
Orientel Aromatics	Camphor, racemic	192762009	1
Phoenix	Camphor, racemic	192762002	1
Phönix	Camphor, racemic	183279002	1
Phönix	Camphor, racemic	21002072002	1
Sanacorp	Camphor, racemic	18327903	1
Sanacorp	Camphor, racemic	21000070026	1

- 235 705 spectra from 1515 *Apo-Ident* customers from a total of 49 200 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Camphor, racemic/D-Camphor* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Camphor, racemic/D-Camphor* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	480	0	152 482
Type B	0	500	0	201 584
Type C	0	361	1	234 979

The substance/substance group *Camphor, racemic/D-Camphor* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8000 %)
Type C	100.0000 % (> 99.9005 %)	99.7238 % (> 98.8950 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24680	24680	0.00	170.44
25048	24680	11.27	171.04
25049	25562	11.13	170.60
25050	27262	9.14	170.05
25051	25051	0.00	168.33
25053	24680	10.05	169.71
25562	25562	0.00	168.93
25977	24680	35.84	162.72
27091	25562	19.44	169.59
27262	27262	0.00	167.46

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cannabidiol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	22416-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cannabidiol

Special notes

When selecting the *Cannabidiol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cannabidiol	7	6	261

Second-stage model

For differentiation of the substance/substance group *Cannabidiol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cannabidiol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Estriol	98.95	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cannabidiol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cannabidiol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cannabidiol	21000530	25612	40	20210218*
Caelo	Cannabidiol	21000530	25612SI	40	20210218*
Caelo	Cannabidiol	21003190	25995	40	20211022*
Caelo	Cannabidiol	21003190	25995SI	40	20211022*
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22412	60	1316Q-07806
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22412SI	60	1316Q-07806
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22413	60	1316Q-07806
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22414	60	1316Q-07806
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22415	60	1316Q-07806
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22416	60	1316Q-07806
THC-Pharma GmbH	Cannabidiol	CBD-API17-003	23398	40	20170609
THC-Pharma GmbH	Cannabidiol	CBD-API17-003	23399	40	20170609
THC-Pharma GmbH	Cannabidiol	CBD-API16-003	23464	40	2017B-03911
THC-Pharma GmbH	Cannabidiol	CBD-API16-004	23465	40	2017A-03911
THC-Pharma GmbH	Cannabidiol	H230.320-1	25504	40	20200806
THC-Pharma GmbH	Cannabidiol	H230.320-1	25504SI	40	20200806

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 760 spectra of 16 reference samples from the substance/substance group *Cannabidiol*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 202 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 871 spectra of 20 reference samples from the substance/substance group *Cannabidiol*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
ADREXpharma GmbH	Cannabidiol	19Y21746	26024	40
Caelo	Cannabidiol	21002319	25998	40
Caelo	Cannabidiol	22001216	26110	40
Caelo	Cannabidiol	23002758005	27193	40
THC-Pharma GmbH	Cannabidiol	CBDAPI1801	23929	40
THC-Pharma GmbH	Cannabidiol	H150.920-1	25730	40
ADREXpharma GmbH	Cannabidiol	19Y21746	26024SI	40
Caelo	Cannabidiol	21002319	25998SI	40
Caelo	Cannabidiol	22001216	26110SI	40
Caelo	Cannabidiol	23002758005	27193SI	40
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22413SI†	60
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22414SI†	60
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22415SI†	60
THC-Pharma GmbH	Cannabidiol	15-7221-80338	22416SI†	60
THC-Pharma GmbH	Cannabidiol	CBD-API17-003	23398SI†	40
THC-Pharma GmbH	Cannabidiol	CBD-API17-003	23399SI†	31
THC-Pharma GmbH	Cannabidiol	CBD-API16-003	23464SI†	40
THC-Pharma GmbH	Cannabidiol	CBD-API16-004	23465SI†	40
THC-Pharma GmbH	Cannabidiol	CBDAPI1801	23929SI	40
THC-Pharma GmbH	Cannabidiol	H150.920-1	25730SI	40

- 201 213 spectra from a total of 4035 batches from further 838 substances. These spectra were

recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1707 spectra from 179 *Apo-Ident* customers from 290 batches from the substance/substance group *Cannabidiol*.
- Among them are spectra of independent samples from 213 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cannabidiol	10C120722-0	1
	Cannabidiol	22001216008	3
	Cannabidiol	23167A	1
	Cannabidiol	23230C	1
	Cannabidiol	23231B	1
	Cannabidiol	23274B	1
	Cannabidiol	23N9251	1
	Cannabidiol	ACPN920903	1
	Cannabidiol	CA215062024	2
	Cannabidiol	CA216062024	1
	Cannabidiol	CBD2102A01	1
	Cannabidiol	CBD2105A02	1
	Cannabidiol	CBDAPI2102	1
	Cannabidiol	G23ACV-ICS1	3
	Cannabidiol	G23ACV-ICS2	1
	Cannabidiol	KI0001	1
	Cannabidiol	KI0002	1
	Cannabidiol	KI0003	2
	Cannabidiol	KI0006	1
	Cannabidiol	KI0007	1
	Cannabidiol	KI0011	1
	Cannabidiol	KI0018	2
	Cannabidiol	KI0021	2
	Cannabidiol	LL130122022	2
	Cannabidiol	LL148032023	6
	Cannabidiol	LL164062023	1
	Cannabidiol	LL165062023	1
	Cannabidiol	LL166062023	1
	Cannabidiol	LL167062023	1
	Cannabidiol	LL181092023	3
	Cannabidiol	LL186102023	2
	Cannabidiol	LL198012024	1
	Cannabidiol	l174122021	1
	Cannabidiol	LL86022022	1
Adex Pharma	Cannabidiol	100493	1
Adrex / AH	Cannabidiol	100492	1
Adrex / Alli. HC	Cannabidiol	100505	1
Adrex / Anzag	Cannabidiol	100493	1
Adrex / Gehe	Cannabidiol	100492	1
Adrex / Gehe	Cannabidiol	100493	2
Adrex / Gehe	Cannabidiol	100505	2

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Adrex / Gehe	Cannabidiol	100506	1
Adrex / Gehe	Cannabidiol	19Y21748	1
Adrex / Jenne	Cannabidiol	100504	1
Adrex / Jenne	Cannabidiol	100505	1
Adrex / Jenne	Cannabidiol	19Y21746	5
Adrex / Jenne	Cannabidiol	LL118092022	1
Adrex / Jenne	Cannabidiol	LL35072021	2
Adrex / Jenne	Cannabidiol	LL61102021	4
Adrex / Jenne	Cannabidiol	LL74122021	5
Adrex / Jenne	Cannabidiol	LL75122021	1
ADREX / Sana	Cannabidiol	100441	1
ADREX / Sana	Cannabidiol	100462	1
Adrex / Sanacorp	Cannabidiol	100462	1
Adrex /Gehe 07.03.22...	Cannabidiol	LL50092021	1
Adrex /Gehe 17.09.21	Cannabidiol	LL31072021	1
Adrex /Phönix 14.03....	Cannabidiol	LL137022023	1
Adrex gEHE	Cannabidiol	100461	1
adrex Gehe	Cannabidiol	100462	1
Adrex pharm	Cannabidiol	100461	2
Adrex pharm	Cannabidiol	100462	2
Adrex pharm	Cannabidiol	100506	1
Adrex Pharm	Cannabidiol	100506	1
Adrex pharm	Cannabidiol	100578	1
adrex pharm	Cannabidiol	13956-29-1	1
Adrex Pharma / AHD 2...	Cannabidiol	100505	1
Adrex Pharma / AHD	Cannabidiol	LL35072021	1
Adrex Pharma / Phoenix	Cannabidiol	LL115082022	1
Adrex Pharma / Phoenix	Cannabidiol	LL62102021	1
Adrex Pharma / Phoenix	Cannabidiol	LL63102021	1
Adrex Pharma / Sanacorp	Cannabidiol	19Y21748	2
Adrex Pharma GmbH	Cannabidiol	100462	1
Adrex Pharma GmbH	Cannabidiol	1133072021	1
Adrex Pharma GmbH	Cannabidiol	LL33072021	1
Adrex Pharma/ Gehe	Cannabidiol	LL50092021	1
Adrex Pharma/ Jenne	Cannabidiol	LL74122021	3
Adrex Pharma/ Noweda	Cannabidiol	100506	1
Adrex Pharma/ Noweda	Cannabidiol	19Y21748	1
Adrex Pharma/ Phönix	Cannabidiol	100506	1
Adrex Pharma/ Phönix	Cannabidiol	LL63102021	1
Adrex Pharma/ Sanacorp	Cannabidiol	100492	2
Adrex Pharma/4	Cannabidiol	100442	1
Adrex Pharma/AEP	Cannabidiol	100440	1
Adrex Pharma/Jenne	Cannabidiol	LL62102021	1
Adrex Pharma/Noweda	Cannabidiol	100442	1
Adrex Pharma/Noweda	Cannabidiol	100462	1
Adrex pharma/Sanacorp	Cannabidiol	LL32072021	1
adrex Pharma	Cannabidiol	100442	2
ADREX pharma	Cannabidiol	100460	2
Adrex Pharma	Cannabidiol	100461	1
Adrex Pharma	Cannabidiol	100492	2
Adrex Pharma	Cannabidiol	100505	3
adrex pharma	Cannabidiol	100506	1
Adrex pharma	Cannabidiol	19Y21746	4
Adrex Pharma	Cannabidiol	19Y21746	1
Adrex Pharma	Cannabidiol	19Y21748	2
Adrex Pharma	Cannabidiol	LL50092021	1
Adrex pharma	Cannabidiol	LL61102021	2
Adrex Pharma	Cannabidiol	LL75122021	1
ADREX/ Jenne	Cannabidiol	100504	1
Adrex/AEP	Cannabidiol	100493	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Adrex/AHD	Cannabidiol	LL115082022	1
Adrex/AHD	Cannabidiol	LL117092022	1
Adrex/AHD	Cannabidiol	LL120102022	1
Adrex/AHD	Cannabidiol	LL97042022	1
Adrex/Anzag	Cannabidiol		1
Adrex/Anzag	Cannabidiol	10(100492)	1
Adrex/Anzag	Cannabidiol	100440	1
Adrex/Anzag	Cannabidiol	11(100492)	1
Adrex/Anzag	Cannabidiol	12(100492)	1
Adrex/Anzag	Cannabidiol	13(100505)	1
Adrex/Anzag	Cannabidiol	14(100492)	1
Adrex/Anzag	Cannabidiol	220504(LL61102021)	1
Adrex/Gehe	Cannabidiol	100461	1
Adrex/Gehe	Cannabidiol	LL62102021	1
Adrex/Gehe	Cannabidiol	LL75122021	5
Adrex/Gehe	Cannabidiol	LL97042022	3
Adrex/Jenne	Cannabidiol	211020(LL35072021)	1
Adrex/Jenne	Cannabidiol	220110(19Y21746)	1
Adrex/Jenne	Cannabidiol	220307(LL61102021)	1
Adrex/Jenne	Cannabidiol	220428(LL61102021)	1
Adrex/Jenne	Cannabidiol	220715(LL97042022)	1
Adrex/Jenne	Cannabidiol	LL35072021	1
Adrex/Noweda 20.10.2021	Cannabidiol	LL35072021	1
Adrex/Noweda	Cannabidiol	100441	2
Adrex/Noweda	Cannabidiol	100460	3
Adrex/Noweda	Cannabidiol	100461	2
Adrex/Noweda	Cannabidiol	100493	1
Adrex/Noweda	Cannabidiol	100504	1
Adrex/Phoenix	Cannabidiol	100462	1
Adrex/Phoenix	Cannabidiol	LL110072022	2
Adrex/Phön 07.11.22 …	Cannabidiol	LL115082022	1
Adrex/Phön 6.01.23 E…	Cannabidiol	LL120102022	1
Adrex/Phönix 02.09.2…	Cannabidiol	LL110072022	1
Adrex/Phönix 12.07.2…	Cannabidiol	LL97042022	1
Adrex/Phönix 17.05.2…	Cannabidiol	LL75122021	1
Adrex/Phönix	Cannabidiol	100493	1
Adrex/Phönix	Cannabidiol	100505	2
Adrex/Phönix	Cannabidiol	LL35072021	2
Adrex/Phönix	Cannabidiol	LL61102021	2
Adrex/Sanacorp	Cannabidiol	100441	1
Adrex/Sanacorp	Cannabidiol	100460	4
Adrex	Cannabidiol	100442	2
Adrex	Cannabidiol	100491	1
Adrex	Cannabidiol	100505	1
ADREX	Cannabidiol	100505	1
Adrex	Cannabidiol	19Y21746	2
Adrex	Cannabidiol	LL117092022	1
Adrex	Cannabidiol	LL130122022	1
Adrex	Cannabidiol	LL35072021	1
adrex	Cannabidiol	LL48092021	1
adrex	Cannabidiol	LL49092021	1
Adrex	Cannabidiol	LL49092021	1
Adrex	Cannabidiol	LL61102021	2
adrex	Cannabidiol	LL62102021	1
Adrex	Cannabidiol	LL63102021	1
Adrex	Cannabidiol	LL75122021	2
Adrex	Cannabidiol	LL82012022	1
adrex	Cannabidiol	l184022022	1
Adrexa/Jenne	Cannabidiol	19Y21746	1
Adrex-Noweda	Cannabidiol	100505	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
ADREXpharma - Sanacorp	Cannabidiol	100441	1
Adrexpharma / Sanacorp	Cannabidiol	100461	1
ADREXpharma GmbH/Phönix	Cannabidiol	19Y21746	3
ADREXpharma GmbH	Cannabidiol	100400	1
ADREXpharma GmbH	Cannabidiol	100442	1
ADREXpharma GmbH	Cannabidiol	100462	1
ADREXpharma GmbH	Cannabidiol	100491	1
ADREXpharma GmbH	Cannabidiol	100493	2
ADREXpharma GmbH	Cannabidiol	19Y21746	1
adrexpharma GmbH	Cannabidiol	LL114082022	1
adrexpharma GmbH	Cannabidiol	LL117092022	2
adrexpharma GmbH	Cannabidiol	LL120102022	3
ADREXpharma GmbH	Cannabidiol	LL32072021	1
adrexpharma GmbH	Cannabidiol	LL62102021	1
Adrexpharma GmbH	Cannabidiol	LL82012022	1
ADREXpharma, Gehe	Cannabidiol	100491	1
ADREXpharma, Gehe	Cannabidiol	LL48092021	1
Adrexpharma/ Phoenix	Cannabidiol	LL110072022	1
Adrexpharma/ Phoenix	Cannabidiol	LL115082022	2
Adrexpharma/ Phoenix	Cannabidiol	LL117092022	1
Adrexpharma/ Phoenix	Cannabidiol	LL48092021	2
Adrexpharma/ Phoenix	Cannabidiol	LL49092021	2
Adrexpharma/ Phoenix	Cannabidiol	LL62102021	4
Adrexpharma/ Phoenix	Cannabidiol	LL97042022	3
ADREXpharma/ Sanacorp	Cannabidiol	LL32072021	1
Adrexpharma/Gehe	Cannabidiol	LL97042022	2
Adrexpharma/Noweda	Cannabidiol	LL114082022	3
Adrexpharma/Noweda	Cannabidiol	LL115082022	1
Adrexpharma/Noweda	Cannabidiol	LL118092022	1
Adrexpharma/Noweda	Cannabidiol	LL14082022	1
Adrexpharma/Noweda	Cannabidiol	LL50092021	1
Adrexpharma/Noweda	Cannabidiol	LL62102021	3
Adrexpharma/Noweda	Cannabidiol	LL63102021	1
Adrexpharma/Noweda	Cannabidiol	LL7092022	1
Adrexpharma/Noweda	Cannabidiol	LL75122021	2
Adrexpharma/Noweda	Cannabidiol	LL97042022	6
AdrexPharma	Cannabidiol	100442	7
ADREXpharma	Cannabidiol	100442	5
Adrexpharma	Cannabidiol	100460	1
Adrexpharma	Cannabidiol	100461	1
AdrexPharma	Cannabidiol	100462	1
AdrexPharma	Cannabidiol	100493	1
AdrexPharma	Cannabidiol	100506	10
AdrexPharma	Cannabidiol	19Y21746	12
ADREXpharma	Cannabidiol	19Y21746	2
AdrexPharma	Cannabidiol	19Y21748	13
ADREXpharma	Cannabidiol	19Y21748	2
ADREXpharma	Cannabidiol	19Y217848	1
AdrexPharma	Cannabidiol	LL31072021	2
AdrexPharma	Cannabidiol	LL32072021	1
AdrexPharma	Cannabidiol	LL33072021	1
AdrexPharma	Cannabidiol	LL48092021	6
AdrexPharma	Cannabidiol	LL49092021	3
AdrexPharma	Cannabidiol	LL50092021	6
Adrexpharma	Cannabidiol	LL62102021	1
AEP/Adrexpharma Gmbh	Cannabidiol	100492	1
Alliance Healthcare	Cannabidiol	100441	1
Alliance Healthcare	Cannabidiol	100492	2
Alliance Healthcare	Cannabidiol	19Y21748	1
Alliance Healthcare	Cannabidiol	22263A	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Alliance Healthcare	Cannabidiol	22398B	1
Alliance Healthcare	Cannabidiol	KI0007	1
Alliance Healthcare	Cannabidiol	LL181092023	2
Alliance Healthcare	Cannabidiol	LL32072021	1
Alliance Healthcare	Cannabidiol	LL62102021	1
Alliance Healthcare	Cannabidiol	LL75122021	1
alpha -Cannabis Phar...	Cannabidiol	ACPL418001	1
Alpha Cannabis pharm...	Cannabidiol	ACPL418001	1
alpha Cannabis/ApoCa...	Cannabidiol	ACPM810901	6
Alpha Cannabis/Apoca...	Cannabidiol	ACPL418001	1
alpha cannabis	Cannabidiol	ACPL416001	1
alpha-cannabis 09.07.20	Cannabidiol	ACPLO09001P-200709-4	1
alpha-cannabis 10.08.20	Cannabidiol	ACPLO0900P-200810-1	1
alpha-cannabis 31.03.20	Cannabidiol		1
alpha-cannabis Pharm...	Cannabidiol	ACPLO	1
alpha-cannabis Pharm...	Cannabidiol	ACPLO09001	5
alpha-cannabis Pharm...	Cannabidiol	ACPM810901	4
alpha-cannabis Pharm...	Cannabidiol	ACLP416001	1
alpha-cannabis Pharm...	Cannabidiol	ACPK012405	1
alpha-cannabis Pharm...	Cannabidiol	ACPK911004	3
alpha-cannabis Pharm...	Cannabidiol	ACPL416001	3
alpha-cannabis Pharm...	Cannabidiol	ACPLO09001	2
alpha-cannabis Pharm...	Cannabidiol		1
alpha-cannabis Pharm...	Cannabidiol	ACPL418001P190711-1	1
alpha-cannabis Pharm...	Cannabidiol		1
alpha-cannabis Pharm...	Cannabidiol		1
alpha-cannabis Pharm...	Cannabidiol		1
alpha-cannabis Pharm...	Cannabidiol		1
alpha-cannabis Pharm...	Cannabidiol	ACPK012405P190430-2	1
alpha-cannabis Pharm...	Cannabidiol		1
alpha-cannabis Pharm...	Cannabidiol	ACPK012405P190405-1	1
alpha-cannabis Pharm...	Cannabidiol		1
alpha-cannabis Pharm...	Cannabidiol	ACPL418001P-190613-2	1
alpha-cannabis Pharm...	Cannabidiol	ACPK312001	1
alpha-cannabis Pharm...	Cannabidiol	ACPK91100P-181220-1	1
alpha-cannabis Pharm...	Cannabidiol	ACPL41800P-190527-2	1
alpha-cannabis Pharma	Cannabidiol	ACPK312001	2
alpha-cannabis Pharma	Cannabidiol	ACPL416001	2
alpha-cannabis Pharma	Cannabidiol	ACPL418001	2
Alpha-Cannabis Pharma	Cannabidiol	ACPN920903	2
Alpha-Cannabis Pharma	Cannabidiol	ACPP310901	3
Andrex	Cannabidiol	19y21748	1
Anzag/Adrex Pharma	Cannabidiol	100441	5
Anzag/Adrex Pharma	Cannabidiol	100461	8
Anzag/trigal	Cannabidiol	F190205	1
ApoCare GmbH	Cannabidiol	ACPLO09001	11
Apocare Pharma 11.05.20	Cannabidiol		1
Apocare Pharma 15.06.2020	Cannabidiol		1
Apocare Pharma 16.12.19	Cannabidiol	ACPL009001P-191216-1	1
APOCARE Pharma GmbH	Cannabidiol	ACPL416001	3
APOCARE Pharma GmbH	Cannabidiol	ACPL418001	1
Apocare Pharma	Cannabidiol		1
Apocare Pharma	Cannabidiol	ACPL416001	1
Apocare	Cannabidiol	ACPK312001	1
Apocare	Cannabidiol	ACPK911004	9
Apocare	Cannabidiol	ACPL418001	3
Apocare	Cannabidiol	ACPLO09001	1
Ardex / Noweda	Cannabidiol	LL75122021	3
Ardex / Noweda	Cannabidiol	LL97042022	8
Ardex/Noweda	Cannabidiol	19Y21746	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Ardrex PH./Phönix	Cannabidiol	100462	2
Arevipharma GmbH/ Phoenix	Cannabidiol		3
Arevipharma GmbH/ Phoenix	Cannabidiol	100505	5
Arevipharma GmbH/ Phoenix	Cannabidiol	19Y21746	1
BAFA GmbH	Cannabidiol		1
Bombastus	Cannabidiol		1
BSPG Lab. Ltd UK/Can...	Cannabidiol	CKB20ICB4TB	1
BSPG/Pharma line	Cannabidiol	F181001	10
BSPG/Trigal Pharm GmbH	Cannabidiol	FB181001	10
BSPG	Cannabidiol	F200205	1
Caelo	Cannabidiol		14
Caelo	Cannabidiol	110216-02	3
Caelo	Cannabidiol	16992311	1
Caelo	Cannabidiol	21000530001	1
Caelo	Cannabidiol	21001526003	3
Caelo	Cannabidiol	21002318002	1
Caelo	Cannabidiol	21002319002	13
Caelo	Cannabidiol	2100239002	1
Caelo	Cannabidiol	21003190004	1
Caelo	Cannabidiol	22001216003	3
Caelo	Cannabidiol	ACPK911004P181203-1	1
Caelo	Cannabidiol	CBD-API17-003	1
Caelo	Cannabidiol	CBD-API17-006	2
Caelo	Cannabidiol	CBDAPI1801	2
Caelo	Cannabidiol	CBDAPI1803	1
Caelo	Cannabidiol	F190205	1
Caesar & Loretz GmbH...	Cannabidiol	LL97042022	1
Caesar & Loretz GmbH	Cannabidiol	21000530001	8
Caesar & Loretz GmbH	Cannabidiol	21000530003	1
Caesar & Loretz GmbH	Cannabidiol	21001526004	7
Caesar & Loretz GmbH	Cannabidiol	21003190001	5
Caesar & Loretz GmbH	Cannabidiol	22001216007	1
Cannamedical / Phönix	Cannabidiol	CKB20ICB4TB	2
Cannamedical GmbH	Cannabidiol	CKB20ICB35	1
Cannamedical Pharma GmbH	Cannabidiol	ckb20icb35	1
Cannamedical Pharma GmbH	Cannabidiol	CKB20ICB35	1
Cannamedical Pharma GmbH	Cannabidiol	CKB20ICB4TB	1
Cannamedical Pharma GmbH	Cannabidiol	CKB20ICCB4TB	1
Cannamedical Pharma GmbH	Cannabidiol	ckb9icbanc	1
Cannamedical Pharma	Cannabidiol	CKB9ICBANC	5
Cannamedical	Cannabidiol	CKB20ICB4TB	2
Cannamedical	Cannabidiol	CKB9ICBANB	2
CannaMedical	Cannabidiol	CMB21ICB08417	1
CannAMEDICAL	Cannabidiol	CMB21ICB091432	1
Cantourage/AHD	Cannabidiol	22021A	5
Cantourage/Gehe	Cannabidiol	22020A	1
Cantourage/Phönix	Cannabidiol	2021A	1
Cantourage/Phönix	Cannabidiol	22012B	5
Cantourage/Phönix	Cannabidiol	22020A	1
Cantourage	Cannabidiol	22012B	1
CB21 Pharma,s.r.o.	Cannabidiol	LL25032021	1
Direkt Apocare Pharma	Cannabidiol		1
Euro OTC	Cannabidiol		3
Fagron	Cannabidiol	20C12-F51-381419	2
farmako GmbH	Cannabidiol	LL01022020	1
Farmako GmbH	Cannabidiol	LL01022020	1
farmako Gmbh	Cannabidiol	LL02022020	2
Farmbios S.p.A.	Cannabidiol	100461	1
Gehe, Adrex	Cannabidiol	LL32072021	1
Gehe/ ADREX pharma	Cannabidiol	100441	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe/Adrex 21.1.22 E...	Cannabidiol	LL63102021	1
Gehe/Adrex Pharma	Cannabidiol	19Y21746	2
Gehe/Adrex	Cannabidiol	100440	1
Gehe/Arevipharma Gmbh	Cannabidiol	100505	1
Gehe	Cannabidiol	23230C	1
Gehe	Cannabidiol	LL148032023	1
Gehe	Cannabidiol	LL159052023	1
Gehe	Cannabidiol	LL48092021	1
Gehe	Cannabidiol	LL49092021	1
Hempartis	Cannabidiol	AL18120401	2
Ichtyolgesellschaft ...	Cannabidiol	CA20190508	1
Ilios Sante 01.04.21	Cannabidiol	LL020222020	2
Ilios Sante 2.2.21	Cannabidiol	LL02022020	2
Jenne / Adrex	Cannabidiol	100505	4
Jenne / Adrex	Cannabidiol	19Y21746	2
Jenne / Adrex	Cannabidiol	19Y21748	4
Jenne / Adrex	Cannabidiol	LL120102022	1
Jenne / Adrex	Cannabidiol	LL32072021	1
Jenne / Adrex	Cannabidiol	LL50092021	1
Jenne / Trigal Pharma	Cannabidiol	F190205	1
Jenne / Trigal Pharma	Cannabidiol	F190703E	1
Jenne / Trigal Pharma	Cannabidiol	F190704	1
Jenne	Cannabidiol	ACPN920901	1
Krieger am 5.3.und7....	Cannabidiol	19Y21746	3
Laborchemie APOLDA GmbH	Cannabidiol	APCK312001	1
Noweda/Adrex	Cannabidiol	LL82012022	2
Noweda/THC Pharm	Cannabidiol		6
Noweda	Cannabidiol	100440	1
Noweda	Cannabidiol	100505	2
Noweda	Cannabidiol	16013039	1
Noweda	Cannabidiol	LL164062023	1
Noweda	Cannabidiol	LL181092023	1
Noweda	Cannabidiol	LL62102021	1
Noweda	Cannabidiol	LL72112021	1
Pharmachem GmbH & Co. KG	Cannabidiol		4
Pharmachem GmbH & Co. KG	Cannabidiol	CBDAPI1801	2
Phoenix / Adrexpharma	Cannabidiol	LL63102021	1
Phoenix	Cannabidiol	LL77122021	1
Phönix/THC	Cannabidiol	1C240220-2	1
Phönix	Cannabidiol		1
Phönix	Cannabidiol	19Y21747	1
Sanacorp /Adrex Pharma	Cannabidiol	100441	2
Sanacorp Stralsund	Cannabidiol	LL63102021	1
Sanacorp/Adrex	Cannabidiol	100461	1
Sanacorp	Cannabidiol		6
Sanacorp	Cannabidiol	CBDAPI1804	3
Sanum	Cannabidiol	22020A	3
SANUM-Kehlbeck GmbH&Co.KG	Cannabidiol	22397A	1
SANUM-Kehlbeck/AHD	Cannabidiol	22263A	3
SANUM-Kehlbeck/AHD	Cannabidiol	22398B	4
SANUM-Kehlbeck/Phönix	Cannabidiol	22262B	1
Sanum-Kehlbeck	Cannabidiol	22020A	1
SolMic BioTechGmbH	Cannabidiol	100492	3
Spectrum Therapeutics	Cannabidiol	CBD2105A02	2
Spectrum Therapeutis...	Cannabidiol	CBD2105A02	1
Spectrum Therapeutis...	Cannabidiol	VC2002-007	1
Spectrum	Cannabidiol		1
Sterling Pharma/ Phoenix	Cannabidiol	LL32072021	7
Sterling Pharma	Cannabidiol	LL35072021	1
THC Pharm / THC Pharm	Cannabidiol		1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
THC Pharm GmbH / THC…	Cannabidiol	CBD-API17-005	1
THC Pharm GmbH The …	Cannabidiol		4
THC Pharm GmbH/Noweda	Cannabidiol	10C080421-3	4
THC Pharm GmbH/Noweda	Cannabidiol	10C090421-2	1
THC Pharm GmbH/Noweda	Cannabidiol	10C150121-1	3
THC Pharm GmbH/Noweda	Cannabidiol	10C150321-1	2
THC Pharm GmbH/Noweda	Cannabidiol	10C150321-2	2
THC Pharm GmbH/Noweda	Cannabidiol	10C150321-3	3
THC Pharm GmbH/Phönix	Cannabidiol		2
THC Pharm GmbH/Phönix	Cannabidiol	10C080421-1	1
THC Pharm GmbH/Phönix	Cannabidiol	10C150321-1	1
THC Pharm GmbH/Phönix	Cannabidiol	10C160321-2	1
thc pharm gmbh	Cannabidiol		3
THC Pharm GmbH	Cannabidiol		94
THC Pharm GmbH	Cannabidiol	100493	1
THC Pharm GmbH	Cannabidiol	10C041219-0	1
THC Pharm GmbH	Cannabidiol	10C121119-2	1
THC Pharm GmbH	Cannabidiol	10C180520	1
THC Pharm GmbH	Cannabidiol	10C180520-0	3
THC Pharm GmbH	Cannabidiol	1C031219-0	5
THC Pharm GmbH	Cannabidiol	CBD-API17-005	3
THC Pharm GmbH	Cannabidiol	CBD-API17-006	2
THC Pharm GmbH	Cannabidiol	CBDAPI1707	2
THC Pharm GmbH	Cannabidiol	CBDAPI1801	3
THC Pharm GmbH	Cannabidiol	CBDAPI1802	1
THC Pharm GmbH	Cannabidiol	CBDAPI1804	2
THC Pharm GmbH	Cannabidiol	CBDAPI1805	5
THC Pharm GmbH	Cannabidiol	S20-017	1
THC Pharm/ direkt	Cannabidiol		8
THC Pharm/ Noweda	Cannabidiol		2
THC Pharm/ THC Pharm GmbH	Cannabidiol		1
THC Pharm/ THC Pharm	Cannabidiol		2
THC Pharm/AHD	Cannabidiol		1
THC PHARM/GEHE	Cannabidiol		2
THC Pharm/Phönix	Cannabidiol		2
THC Pharm/THC Pharma	Cannabidiol		1
Thc Pharm	Cannabidiol		1
THC Pharm	Cannabidiol		126
THC PHARM	Cannabidiol		1
THC Pharm	Cannabidiol	10C140819-1	1
THC Pharm	Cannabidiol	10C170619-1	1
THC Pharm	Cannabidiol	CA20190507_01	1
THC Pharm	Cannabidiol	CA20190508_01	1
THC Pharm	Cannabidiol	CA20190508_02	1
THC PHARM	Cannabidiol	CBD2006A01	1
THC PHARM	Cannabidiol	CBD2007A03	1
THC PHARM	Cannabidiol	CBD2107A02	1
THC Pharm	Cannabidiol	CBD-API16-004	6
THC Pharm	Cannabidiol	CBD-API17-004	1
THC Pharm	Cannabidiol	CBD-API17-006	2
THC Pharm	Cannabidiol	CBDAPI1707	1
THC Pharm	Cannabidiol	CBDAPI1708	2
THC Pharm	Cannabidiol	CBDAPI1802	2
THC Pharm	Cannabidiol	CBDAPI1804	5
THC Pharm	Cannabidiol	CBDAPI1901	1
THC Pharm	Cannabidiol	CBDAPL1802	1
THC Pharm	Cannabidiol	H150218-1	1
THC Pharma (direkt)	Cannabidiol		2
THC Pharma (direkt)	Cannabidiol	CBD-API17-006	1
THC Pharma (direkt)	Cannabidiol	CBDAPI1707	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
THC Pharma (direkt)	Cannabidiol	CBDAPI1708	1
THC Pharma (direkt)	Cannabidiol	CBDAPI1801	1
THC Pharma / Cansati...	Cannabidiol		5
THC PHARMA GMBH	Cannabidiol	1C010420-2	1
THC Pharma/ Phönix	Cannabidiol		23
THC Pharma/ Phönix	Cannabidiol	10C060421-0	3
THC Pharma/ THC Pharma	Cannabidiol		1
Thc Pharma/Gehe	Cannabidiol		6
THC Pharma/Gehe	Cannabidiol		1
THC Pharma/Noweda	Cannabidiol		1
THC Pharma/Noweda	Cannabidiol	10C250220-1	1
THC Pharma/Phönix	Cannabidiol		36
THC Pharma/Phönix	Cannabidiol	10C010420-2	4
THC Pharma/Phönix	Cannabidiol	10C180520-0	1
THC Pharma/Phönix	Cannabidiol	10C300320-3	4
THC Pharma/THC Pharma	Cannabidiol		2
THC pharma	Cannabidiol		3
THC Pharma	Cannabidiol		234
THC Pharma	Cannabidiol	10C180520-0	2
THC Pharma	Cannabidiol	1C210619-1	6
THC Pharma	Cannabidiol	CBD2108A02	1
THC Pharma	Cannabidiol	CBDAP/1801	1
THC Pharma	Cannabidiol	CBD-API16-004	3
THC Pharma	Cannabidiol	CBD-API17-002	5
THC Pharma	Cannabidiol	CBD-API17-004	9
THC Pharma	Cannabidiol	CBD-API17-005	6
THC Pharma	Cannabidiol	CBDAPI1706	4
THC Pharma	Cannabidiol	CBDAPI1707	2
THC Pharma	Cannabidiol	CBDAPI1802	4
THC Pharma	Cannabidiol	CBDAPI1803	1
THC Pharma	Cannabidiol	CBDAPI1804	6
THC Pharma	Cannabidiol	CBDAPI1901	3
THC Pharma	Cannabidiol	CBDAPI2003	1
THC Pharma	Cannabidiol	CBDAPI2008	1
THC PHRMA	Cannabidiol		18
THC PHRMA	Cannabidiol	1C090519-1	1
THC Spectrum	Cannabidiol		4
THC/ Direkt	Cannabidiol	CBDAPI1706	1
THC/ THC	Cannabidiol		2
THC/Gehe	Cannabidiol	CBD-API17-005	1
THC/THC	Cannabidiol		2
THC	Cannabidiol		47
THC	Cannabidiol	10C150321-1	1
THC	Cannabidiol	14295559	1
THC	Cannabidiol	CBD-API17-002	2
THC	Cannabidiol	CBD-API17-003	1
THC	Cannabidiol	CBD-API17-004	4
THC	Cannabidiol	CBD-API17-006	2
Thcph	Cannabidiol		1
THC-Pharm/Phoenix	Cannabidiol		1
THC-Pharm	Cannabidiol		13
THC-Pharm	Cannabidiol	cbd-adi17-002	1
THC-Pharm	Cannabidiol	CBDAP/17-003	3
THC-Pharm	Cannabidiol	CBD-API17-004	1
THC-Pharm	Cannabidiol	CBD-API17-005	1
THC-Pharma GmbH	Cannabidiol		7
THC-Pharma	Cannabidiol		21
THC-PHARMA	Cannabidiol	1C140819-0	5
THC-Pharma	Cannabidiol	CBDAP/1708	1
THC-Pharma	Cannabidiol	CBD-API17-003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
THC-Pharma	Cannabidiol	CBDAPI1708	1
THC-Pharma	Cannabidiol	CBDAPI1802	1
THC-Pharma	Cannabidiol	CBDAPI1804	1
THC-Pharma	Cannabidiol	CBDAPI1904	1
TRIGAL Pharma GmbH	Cannabidiol	F200205	1
Trigal Pharma	Cannabidiol	F200205	1
Trigal/Gehe	Cannabidiol	F190205K	11
Trigal/Gehe	Cannabidiol	F200205	10
Trigal/Gehe	Cannabidiol	F200208	6
Trigal/Gehe	Cannabidiol	F200701	31
Trigal/Phoenix	Cannabidiol	F190205	11
Trigal/Phoenix	Cannabidiol	F190704	8

- 234 360 spectra from 1515 *Apo-Ident* customers from a total of 48 969 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cannabidiol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cannabidiol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	760	0	152 202
Type B	0	871	0	201 213
Type C	0	1705	2	234 360

The substance/substance group *Cannabidiol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.2105 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.3111 %)
Type C	100.0000 % (> 99.9007 %)	99.8828 % (> 99.7071 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22412	22412	0.00	99.83
22413	22413	0.00	100.15
22414	22414	0.00	100.26
22415	22415	0.00	100.22
22416	22416	0.00	99.66
23398	22413	6.37	100.21
23399	23465	7.46	100.71
23464	23464	0.00	101.82
23465	23465	0.00	98.95
25504	22415	8.06	100.74
25612	25612	0.00	102.68
25995	25995	0.00	102.55

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Capsaicin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20854-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Capsaicin; Capsacinum

Special notes

When selecting the *Capsaicin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Capsaicin	6	5	14

Second-stage model

For differentiation of the substance/substance group *Capsaicin* the following second-stage model is used:

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Capsaicin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	55.17	–
⋮	⋮	⋮
Alfatradiol	>50	55.29
Sodium citrate	>50	114.99
Levocarnitine	>50	231.46
Prednicarbate	>50	257.71
Oxybutynin hydrochloride	>50	264.49
Tetracaine	>50	276.62
Norethisterone acetate	>50	369.35
Heparin sodium	>50	373.66
Quinine hydrochloride dihydrate	>50	386.48
Cyproterone acetate	>50	454.03
Pyridoxal-5-phosphate	>50	493.33
Methoxsalen	>50	730.08
Ciprofloxacin hydrochloride	>50	846.81
Amifampridine	>50	897.27
Amitriptyline hydrochloride	>50	999.16
Sucrose	>50	1242.77
Triclosan	>50	1381.59
Valine	>50	1550.48

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Capsaicin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Capsaicin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Capsaicin	118066-04	21638	60	20140227
Euro OTC	Capsaicin	1703023	23145	40	20170407*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Capsaicin	1811009	24331	40	20181207*
Euro OTC	Capsaicin	2003046	25258	40	20200701*
Fagron	Capsaicin	13D12-N01	20854	40	1411392
Fagron	Capsaicin	13J07-N07	21340	40	AR-15-FG-007151-01

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 6 reference samples from the substance/substance group *Capsaicin*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.
- 152 702 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 260 spectra of 7 reference samples from the substance/substance group *Capsaicin*.
- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Capsaicin	1603005-01	22930	40
Euro OTC	Capsaicin	1806013-01	24186	40
Euro OTC	Capsaicin	1812015	24457	40
Euro OTC	Capsaicin	1903032	24638	40
Euro OTC	Capsaicin	2312006	27296	40
Euro OTC	Capsaicin	1603005-01	22931	40
Euro OTC	Capsaicin	2312006	27296SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 824 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 47 spectra from 31 *Apo-Ident* customers from 14 batches from the substance/substance group *Capsaicin*.
- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Capsaicin	2003046-03	2
Caelo	Capsaicin	1603005-01	1
Caelo	Capsaicin	180601301	1
EuRho/Alliance Healthcare	Capsaicin	2003046-02	1
EuRho	Capsaicin	1703023-02	1
Euro OTC	Capsaicin	1401043-02	2
Euro OTC	Capsaicin	1603005-01	14
Euro OTC	Capsaicin	1703023-02	1
Euro OTC	Capsaicin	1703023-025346	1
Euro OTC	Capsaicin	1806013-01	2
Euro OTC	Capsaicin	1812015-01	2
Euro OTC	Capsaicin	1903032-02	5
Euro OTC	Capsaicin	19H029	1
Euro OTC	Capsaicin	2003046-02	5
Euro OTC	Capsaicin	I1812015-01	1
Euro OTC	Capsaicin	II1812015-01	1
Extraktion	Capsaicin	2003046-02	1
Fagron	Capsaicin	CP-12003	1
Gehe	Capsaicin	2003046-02	3
Noweda	Capsaicin	2003046-02	1

- 236 020 spectra from 1515 *Apo-Ident* customers from a total of 49 244 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Capsaicin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Capsaicin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	260	0	201 824
Type C	0	46	1	236 020

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The substance/substance group *Capsaicin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.6923 %)
Type C	100.0000 % (> 99.9007 %)	97.8723 % (> 91.4894 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20854	20854	0.00	109.54
21340	21340	0.00	121.89
21638	21340	14.09	137.25
23145	23145	0.00	109.90
24331	24331	0.00	133.89
25258	25258	0.00	105.86

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Captopril**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20890-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Captopril; Captoprilum

Special notes

When selecting the *Captopril* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Captopril	6	7	182

Second-stage model

For differentiation of the substance/substance group *Captopril* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Captopril* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	69.86	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Captopril* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Captopril*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Captopril	12339610	21064	40	1403227
Caelo	Captopril	15189502	21874	60	AR-15-FG-014855-01
Caelo	Captopril	190118	24546	40	20190312*
Fagron	Captopril	12G25-N08	20890	40	20120814
Fagron	Captopril	14B26-B01-312221	21921	60	20140317
Fagron	Captopril	19I24-F01-369346	25370	40	20191031
Fagron	Captopril	19I24-F01-369346	25370SI	40	20191031

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 320 spectra of 7 reference samples from the substance/substance group *Captopril*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 620 spectra of 15 reference samples from the substance/substance group *Captopril*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Captopril	170772	23366	40
Caelo	Captopril	172102	23676	40
Caelo	Captopril	21001156009	25932	40
Caelo	Captopril	23002616	27225	40
Caelo	Captopril	22004035	27229	30
Fagron	Captopril	17G21-B02-337989	23588	30
Fagron	Captopril	22C03-B01-220899	26380	40
Caelo	Captopril	15189502	21874SI†	60
Caelo	Captopril	170772	23366SI	40
Caelo	Captopril	190118	24546SI†	40
Caelo	Captopril	21001156009	25932SI	40
Caelo	Captopril	23002616	27225SI	40
Caelo	Captopril	22004035	27229SI	40
Fagron	Captopril	14B26-B01-312221	21921SI†	60
Fagron	Captopril	22C03-B01-220899	26380SI	40

- 201 464 spectra from a total of 4035 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 673 spectra from 241 *Apo-Ident* customers from 190 batches from the substance/substance group *Captopril*.

- Among them are spectra of independent samples from 181 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Captopril		1
	Captopril	21001156002	1
	Captopril	21003880005	1
	Captopril	21003880009	1
	Captopril	2100388001	1
	Captopril	21003880010	1
	Captopril	22004035001	1
	Captopril	22004035002	12
	Captopril	22004035006	3
	Captopril	22C03-B01	1
	Captopril	22C03-B01-220899	1
	Captopril	22C03-B01-230379	1
	Captopril	23002616002	1
	Captopril	EC220112	1
AHC	Captopril	23002616001	1
AHD	Captopril	22004035001	1
AHD	Captopril	22004035003	1
AHD	Captopril	23002616002	1
Bombastus	Captopril	17210202	1
Caelo	Captopril	12339602	1
Caelo	Captopril	12339604	2
Caelo	Captopril	12339605	4
Caelo	Captopril	12339610	2
Caelo	Captopril	12339616	2
Caelo	Captopril	12339617	1
Caelo	Captopril	12339619	1
Caelo	Captopril	12F29-N04	1
Caelo	Captopril	12G25-N08	2
Caelo	Captopril	14196901	1
Caelo	Captopril	14196903	2
Caelo	Captopril	14196904	8
Caelo	Captopril	14196905	3
Caelo	Captopril	14B26-B01-291555	1
Caelo	Captopril	14B26-B01-291557	1
Caelo	Captopril	14B26-B01-310127	2
Caelo	Captopril	14B26-B40	1
Caelo	Captopril	14B26-B40-318894	1
Caelo	Captopril	14B26-B40-320183	1
Caelo	Captopril	14B26-B40-323267	2
Caelo	Captopril	14B26-B40-325275	2
Caelo	Captopril	14B26-B01-310127	1
Caelo	Captopril	15189501	6
Caelo	Captopril	15189502	1
Caelo	Captopril	15189503	1
Caelo	Captopril	15189504	1
Caelo	Captopril	15189509	3
Caelo	Captopril	15189510	2
Caelo	Captopril	15189511	5
Caelo	Captopril	15189512	11
Caelo	Captopril	15189514	6
Caelo	Captopril	15189514I-041016	1
Caelo	Captopril	15189514I-041016-2	1
Caelo	Captopril	15189515	3
Caelo	Captopril	15189517	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Captopril	15189519	2
Caelo	Captopril	15189521	5
Caelo	Captopril	15189524	2
Caelo	Captopril	15189525	2
Caelo	Captopril	15189526	2
Caelo	Captopril	1519521	1
Caelo	Captopril	16B26-B01310127	1
Caelo	Captopril	17077201	5
Caelo	Captopril	17077202	4
Caelo	Captopril	17077203	1
Caelo	Captopril	17077205	1
Caelo	Captopril	17077206	1
Caelo	Captopril	17077208	8
Caelo	Captopril	17077209	18
Caelo	Captopril	1718A-03358	1
Caelo	Captopril	17210201	6
Caelo	Captopril	17210202	16
Caelo	Captopril	17210203	1
Caelo	Captopril	17210204	5
Caelo	Captopril	17210205	10
Caelo	Captopril	17G27-B02	3
Caelo	Captopril	17G27-B02-340798	1
Caelo	Captopril	17G27-B02-342412	1
Caelo	Captopril	17G27-B02-354613	1
Caelo	Captopril	1805005	1
Caelo	Captopril	18058001	1
Caelo	Captopril	18058002	8
Caelo	Captopril	18058003	1
Caelo	Captopril	18058004	6
Caelo	Captopril	18058005	10
Caelo	Captopril	18058006	3
Caelo	Captopril	18058007	2
Caelo	Captopril	18058009	1
Caelo	Captopril	18058010	2
Caelo	Captopril	19000652002	5
Caelo	Captopril	190006520020	1
Caelo	Captopril	19000652004	9
Caelo	Captopril	19000652005	23
Caelo	Captopril	190115001	1
Caelo	Captopril	190118001	8
Caelo	Captopril	19011801	7
Caelo	Captopril	19011802	4
Caelo	Captopril	19011803	2
Caelo	Captopril	19011805	2
Caelo	Captopril	19011806	4
Caelo	Captopril	19011807	10
Caelo	Captopril	21000272002	3
Caelo	Captopril	21001156001	3
Caelo	Captopril	21001156002	14
Caelo	Captopril	21001156003	1
Caelo	Captopril	21001156005	2
Caelo	Captopril	21001156006	1
Caelo	Captopril	21001156007	5
Caelo	Captopril	21001156009	9
Caelo	Captopril	21001156010	3
Caelo	Captopril	21003880001	8
Caelo	Captopril	21003880002	2
Caelo	Captopril	21003880005	2
Caelo	Captopril	21003880006	10
Caelo	Captopril	21003880007	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Captopril	21003880009	3
Caelo	Captopril	21003880010	1
Caelo	Captopril	21003880011	2
Caelo	Captopril	2100388006	1
Caelo	Captopril	2100388009	1
Caelo	Captopril	22004035001	1
Caelo	Captopril	5102-14-042	1
Caelo	Captopril	901180021	1
Caeol/ Noweda	Captopril	15189519	1
Caeol/ Noweda	Captopril	17077202	1
Caesar & Loretz GmbH...	Captopril	19000652002	1
Caesar & Loretz GmbH...	Captopril	19011802	1
Caesar & Loretz GmbH...	Captopril	21000272002	2
Caesar & Loretz GmbH/Gehe	Captopril	19011805	1
Caesar & Loretz GmbH/Gehe	Captopril	21001156003	1
Caesar & Loretz GmbH...	Captopril	19000652002	1
Caesar & Loretz GmbH...	Captopril	190118002	1
Caesar & Loretz GmbH/Kehr	Captopril	21003880007	1
Caesar & Loretz GmbH/L10	Captopril	21003880002	3
Caesar & Loretz GmbH...	Captopril	21001156002	1
Caesar & Loretz GmbH...	Captopril	19000652002	1
Caesar & Loretz GmbH...	Captopril	21001156006	1
Caesar & Loretz GmbH	Captopril	18058002	1
Caesar & Loretz GmbH	Captopril	18058006	1
Caesar & Loretz GmbH	Captopril	19000652005	3
Caesar & Loretz GmbH	Captopril	19011801	1
Caesar & Loretz GmbH	Captopril	19011802	1
Caesar & Loretz GmbH	Captopril	19011805	2
Caesar & Loretz GmbH	Captopril	19011807	1
Caesar & Loretz GmbH	Captopril	21000272002	1
Caesar & Loretz GmbH	Captopril	21001156002	2
Caesar & Loretz GmbH	Captopril	21001156003	4
Caesar & Loretz GmbH	Captopril	21001156005	1
Caesar & Loretz GmbH	Captopril	21001156007	3
Caesar & Loretz GmbH	Captopril	21001156009	3
Caesar & Loretz GmbH	Captopril	21001156010	2
Caesar & Loretz GmbH	Captopril	21003880001	2
Caesar & Loretz GmbH	Captopril	21003880005	2
Caesar & Loretz GmbH	Captopril	21003880006	2
Caesar & Loretz GmbH	Captopril	21003880007	1
Caesar & Loretz GmbH...	Captopril	19000652005	2
Caesar & Loretz	Captopril	21001156002	1
Caesar&Loretz	Captopril	17210201	1
Cealo/Sanacorp	Captopril	12339617	1
Changzhou Pharmaceutical	Captopril	14B26-B40-321319	1
Euro OTC	Captopril	14B26-B40-320183	1
Euro OTC	Captopril	15189507	3
Euro OTC	Captopril	17210204	1
Euro OTC	Captopril	18058003	1
Euroct/Gehe	Captopril	14B26-B40-320183	1
Fagron	Captopril		1
Fagron	Captopril	12G25-N08	2
Fagron	Captopril	12K16-N04	1
Fagron	Captopril	12K-16N04	1
Fagron	Captopril	1369240	1
Fagron	Captopril	14196902	1
Fagron	Captopril	14B26B01	1
Fagron	Captopril	14B26-B01	6
Fagron	Captopril	14B26-B01_2911557	1
Fagron	Captopril	14B26-B01_302338	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Captopril	14B26-B01-291555	3
Fagron	Captopril	14B26-B01-291556	3
Fagron	Captopril	14B26-B01-291557	5
Fagron	Captopril	14B26-B01-302337	1
Fagron	Captopril	14B26-B01-302338	4
Fagron	Captopril	14B26-B01-310127	6
Fagron	Captopril	14B26-B01-312221	1
Fagron	Captopril	14B26-B01-314460	1
Fagron	Captopril	14B26-B01-316257	2
Fagron	Captopril	14B26-B40-318894	5
Fagron	Captopril	14B26-B40-320183	6
Fagron	Captopril	14B26-B40-321319	5
Fagron	Captopril	14B26B40323267	1
Fagron	Captopril	14B26-B40-323267	3
Fagron	Captopril	14B26-B40-325275	3
Fagron	Captopril	14B26-W0129-1557	1
Fagron	Captopril	17g27-b02-337989	1
Fagron	Captopril	17G27-B02-337989	5
Fagron	Captopril	17G27-B02-340789	1
Fagron	Captopril	17G27-B02-340798	2
Fagron	Captopril	17G27-B02-346203	2
Fagron	Captopril	17G27-B02-350227	1
Fagron	Captopril	17G27-B02-350997	1
Fagron	Captopril	17G27-B02-352730	2
Fagron	Captopril	17G27-B02-356147	6
Fagron	Captopril	17G-B02-352730	1
Fagron	Captopril	19/24-F01	1
Fagron	Captopril	19/24-F01-365391	1
Fagron	Captopril	19/24-F01-367084	1
Fagron	Captopril	19/24-F01-369346	1
Fagron	Captopril	19/24-FO1-367389	1
Fagron	Captopril	19124-F01-3692400	1
Fagron	Captopril	1924-f01-365391	1
Fagron	Captopril	1924-F01-367389	1
Fagron	Captopril	1924F01365391	1
Fagron	Captopril	19I24-F01-365390	2
Fagron	Captopril	19I24-F01-365391	5
Fagron	Captopril	19I24-F01-367084	1
Fagron	Captopril	19I24-F01-367389	1
Fagron	Captopril	19I24-F01-369240	3
Fagron	Captopril	19I24-F01-369345	1
Fagron	Captopril	19I24-F01-369346	3
Fagron	Captopril	19I24-FO1-365391	1
Fagron	Captopril	19l24-F01365391	1
Fagron	Captopril	21/15-B05-2136403	1
Fagron	Captopril	21/15-B05-213643	6
Fagron	Captopril	2115_b05_213643	1
Fagron	Captopril	21I15-B05-213643	4
Fagron	Captopril	21l15-BO5-213643	1
Fagron	Captopril	22003-B01-220899	1
Fagron	Captopril	22C03-B01	2
Fagron	Captopril	22C03-B01-220899	1
Fagron	Captopril	700766	1
Fagron	Captopril	80616-6	1
Fagron	Captopril	EC140101	1
Fagron	Captopril	EC170110	4
Fagron	Captopril	EC18019	1
Fagron	Captopril	EC181019	1
Fagron	Captopril	F01-3653901	1
Fagron	Captopril	F01-3673809	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Captopril	F01-3692400	1
Fagron	Captopril	F01-3693406	1
Fagrron	Captopril	14B26-B01-310127	2
GEHE	Captopril	17077209	1
GEHE	Captopril	17210203	1
Gehe	Captopril	18058002	1
GEHE	Captopril	18058003	1
Gehe	Captopril	18058004	2
Gehe	Captopril	18058010	1
Gehe	Captopril	19011805	2
Gehe	Captopril	21003880009	1
Gehe	Captopril	22C03-B01-234634	1
gepepharm GmbH	Captopril	21003880007	1
Hedinger	Captopril	14B26-B40	2
Herstellung	Captopril	12339607	1
Kehr	Captopril	21003880010	1
Kehr	Captopril	22004035002	3
Klosterring	Captopril	17G27-B02-340471	1
L12	Captopril	17077202	2
Noweda	Captopril	17210202	1
Noweda	Captopril	19011806	1
Noweda	Captopril	21001156009	1
Noweda	Captopril	210388010	1
Noweda	Captopril	22004035001	1
Noweda	Captopril	22004035003	1
Noweda	Captopril	220040358001	1
Noweda	Captopril	22C03-B01-230279	1
Phoenix	Captopril	22004035002	1
Phonix	Captopril	14B26-B01	1
Phönix	Captopril	18058002	1
PHÖNIX	Captopril	19124-f01-367389	1
PHÖNIX	Captopril	19124-f01-369346	2
PHÖNIX	Captopril	19124-f01-63946	1
Phönix	Captopril	2100156002	1
Phönix	Captopril	21003880009	1
Phönix	Captopril	22004035002	1
Sanacorp	Captopril	17077202	1
Sanacorp	Captopril	17077205	1
Sanacorp	Captopril	17210202	1
Sanacorp	Captopril	17G27B02	1
Sanacorp	Captopril	18058004	2
Sanacorp	Captopril	19/24-F01	1
Sanacorp	Captopril	190118001	2
Sanacorp	Captopril	19011806	1
Sanacorp	Captopril	19124-F01-365391	1
Sanacorp	Captopril	19124-F01-367389	3
Sonnenberg-Apotheke	Captopril	14B26-B01-291557	2
THC Pharma	Captopril	18058002	1

- 235 394 spectra from 1515 *Apo-Ident* customers from a total of 49 072 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Captopril* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Captopril* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	620	0	201 464
Type C	0	667	6	235 394

The substance/substance group *Captopril* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0323 %)
Type C	100.0000 % (> 99.9007 %)	99.1085 % (> 98.6627 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20890	21064	6.47	145.40
21064	21064	0.00	145.19
21874	21874	0.00	145.84
21921	21874	10.51	148.93
24546	24546	0.00	142.98
25370	24546	5.38	144.22

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Carbomers**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20548-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Carbomers; Carbomera

Special notes

When selecting the *Carbomers* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Carbomers	12	23	199

Second-stage model

For differentiation of the substance/substance group *Carbomers* the following second-stage model is used:

- Submodel 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Carbomers* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	46.42	42.91
Silver protein	67.12	–
⋮	⋮	⋮
Mg-Ca-K colamine phosphate	>50	93.52
Magnesium citrate	>50	113.33
Gentamicin sulfate	>50	451.79
Tobramycin sulfate	>50	494.45
Finasteride	>50	563.77
Neomycin sulfate	>50	609.38
Zinc gluconate	>50	940.90
Sodium tetraborate	>50	1068.63

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Carbomers* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Carbomers*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Carbomers	13135601	20978	40	1403767
Caelo	Carbomers	13186207	20979	40	1403768
Caelo	Carbomers	14057902	21354	40	20140228
Caelo	Carbomers	14057903	21557	60	20140228
Caelo	Carbomers	162530	22759	40	20161011*
Caelo	Carbomers	21001724	25809	50	20210831*
Caelo	Carbomers	24000748	27218	40	20240419*
Euro OTC	Carbomers	1311027-02	21561	60	20131205
Euro OTC	Carbomers	1512010	22250	60	20151216*
Euro OTC	Carbomers	1604032	22548	40	20160428*
Euro OTC	Carbomers	1607028	22686	40	20160804*
Euro OTC	Carbomers	1610024	22852	40	20161102*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 550 spectra of 12 reference samples from the substance/substance group *Carbomers*. These samples are listed above in the *calibration samples* section. The reference samples come from 12 different batches.
- 152 412 spectra from a total of 2830 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1040 spectra of 28 reference samples from the substance/substance group *Carbomers*.
- Among them are spectra of independent samples from 23 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Carbomers	172520	23621	40
Caelo	Carbomers	173614	23783	40
Caelo	Carbomers	180924	24250	40
Caelo	Carbomers	183074	24543	40
Caelo	Carbomers	190245	24565	40
Caelo	Carbomers	20001190	25227	40
Caelo	Carbomers	21002358	25808	50
Caelo	Carbomers	22002190	26506	40
Caelo	Carbomers	24000213	27227	40
Euro OTC	Carbomers	1702012	23139	40
Euro OTC	Carbomers	1706015	23534	40
Euro OTC	Carbomers	1801044	23959	40
Euro OTC	Carbomers	1810019	24315	40
Euro OTC	Carbomers	1903007	24468	40
Euro OTC	Carbomers	1908029	24858	40
Euro OTC	Carbomers	2003049	25124	40
Euro OTC	Carbomers	2104007	25669	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Carbomers	2112003	25915	40
Euro OTC	Carbomers	2203009	26092	40
Euro OTC	Carbomers	2206008	26195	40
Euro OTC	Carbomers	2302002	26579	40
Euro OTC	Carbomers	2310006	27010	40
Euro OTC	Carbomers	2403011	27200	40
Caelo	Carbomers	24000748	27243	40
Euro OTC	Carbomers	2112003	25915SI	10
Euro OTC	Carbomers	2203009	26092SI	20
Euro OTC	Carbomers	2206008	26195SI	20
Euro OTC	Carbomers	2302002	26579SI	20

- 201 044 spectra from a total of 4021 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 984 spectra from 565 *Apo-Ident* customers from 205 batches from the substance/substance group *Carbomers*.
- Among them are spectra of independent samples from 198 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Carbomers	22002190002	3
	Carbomers	22002190003	4
	Carbomers	23000625003	6
	Carbomers	23002015002	2
	Carbomers	23002015003	1
	Carbomers	23002015004	1
	Carbomers	2302002-01	3
	Carbomers	24000213002	1
Alliance H.	Carbomers	1512010-01	1
Alliance Healthcare	Carbomers	21001724008	1
Anzag	Carbomers	23000625003	1
apo ident	Carbomers	2003049-01	1
Bombastus	Carbomers	18092401	1
Bombastus	Carbomers	22002190003	1
Caeli/sana	Carbomers	21003605001	1
Caelo	Carbomers	10003550042	1
Caelo	Carbomers	1081702	1
Caelo	Carbomers	11013605	2
Caelo	Carbomers	1117I-01232	1
Caelo	Carbomers	11307511	1
Caelo	Carbomers	11351604	1
Caelo	Carbomers	11351605	3
Caelo	Carbomers	11351618	3
Caelo	Carbomers	11351623	1
Caelo	Carbomers	11676321	1
Caelo	Carbomers	12274907	7
Caelo	Carbomers	12274908	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Carbomers	12274910	1
Caelo	Carbomers	12274912	5
Caelo	Carbomers	12274914	3
Caelo	Carbomers	12274916	8
Caelo	Carbomers	12274922	1
Caelo	Carbomers	1311027-02	1
Caelo	Carbomers	13186201	2
Caelo	Carbomers	13186203	3
Caelo	Carbomers	13186205	6
Caelo	Carbomers	13186207	1
Caelo	Carbomers	13194501	5
Caelo	Carbomers	13194503	7
Caelo	Carbomers	13194505	2
Caelo	Carbomers	13194507	4
Caelo	Carbomers	13194511	1
Caelo	Carbomers	13194512	1
Caelo	Carbomers	14016208	7
Caelo	Carbomers	14016209	1
Caelo	Carbomers	14057902	2
Caelo	Carbomers	14057903	2
Caelo	Carbomers	1410001-02	1
Caelo	Carbomers	14149904	2
Caelo	Carbomers	14149905	1
Caelo	Carbomers	14149906	4
Caelo	Carbomers	14149910	2
Caelo	Carbomers	14149911	2
Caelo	Carbomers	15015702	1
Caelo	Carbomers	15015703	1
Caelo	Carbomers	15015709	2
Caelo	Carbomers	15101801	5
Caelo	Carbomers	15101802	6
Caelo	Carbomers	15101807	3
Caelo	Carbomers	15101809	4
Caelo	Carbomers	15101810	5
Caelo	Carbomers	1510801	1
Caelo	Carbomers	15257401	1
Caelo	Carbomers	15257403	1
Caelo	Carbomers	154390002	1
Caelo	Carbomers	15439002	12
Caelo	Carbomers	15439003	11
Caelo	Carbomers	15439004	1
Caelo	Carbomers	1604032-01	2
Caelo	Carbomers	1607028-01	1
Caelo	Carbomers	1610024-01	1
Caelo	Carbomers	162375	1
Caelo	Carbomers	16237501	1
Caelo	Carbomers	162530	1
Caelo	Carbomers	16253001	2
Caelo	Carbomers	16253002	1
Caelo	Carbomers	16253003	1
Caelo	Carbomers	16253004	10
Caelo	Carbomers	16253005	6
Caelo	Carbomers	16253007	10
Caelo	Carbomers	16253009	12
Caelo	Carbomers	16253011	1
Caelo	Carbomers	16253012	7
Caelo	Carbomers	16253014	5
Caelo	Carbomers	17053182	1
Caelo	Carbomers	1706015-01	1
Caelo	Carbomers	17146501	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Carbomers	17361402	11
Caelo	Carbomers	17361403	5
Caelo	Carbomers	18049301	1
Caelo	Carbomers	18049304	1
Caelo	Carbomers	180924006	1
Caelo	Carbomers	18092401	37
Caelo	Carbomers	18092402	4
Caelo	Carbomers	18092403	1
Caelo	Carbomers	18092405	21
Caelo	Carbomers	18092406	6
Caelo	Carbomers	18092408	12
Caelo	Carbomers	18092411	2
Caelo	Carbomers	18092412	2
Caelo	Carbomers	1810024-01	1
Caelo	Carbomers	181016184	1
Caelo	Carbomers	18307401	18
Caelo	Carbomers	18307402	2
Caelo	Carbomers	18307403	6
Caelo	Carbomers	18307406	3
Caelo	Carbomers	18307407	1
Caelo	Carbomers	18307408	14
Caelo	Carbomers	18307410	4
Caelo	Carbomers	18307411	4
Caelo	Carbomers	18307413	2
Caelo	Carbomers	19000614002	2
Caelo	Carbomers	19000614003	1
Caelo	Carbomers	19024505	3
Caelo	Carbomers	19145601	1
Caelo	Carbomers	192276003	5
Caelo	Carbomers	192276004	18
Caelo	Carbomers	19227601	5
Caelo	Carbomers	19227602	12
Caelo	Carbomers	19236601	2
Caelo	Carbomers	2000034003	1
Caelo	Carbomers	20000343001	3
Caelo	Carbomers	20000343003	22
Caelo	Carbomers	20001190002	2
Caelo	Carbomers	20001190003	11
Caelo	Carbomers	200011910003	1
Caelo	Carbomers	2000190003	1
Caelo	Carbomers	2000190008	1
Caelo	Carbomers	20003095003	2
Caelo	Carbomers	20003238001	2
Caelo	Carbomers	20003924001	14
Caelo	Carbomers	20003924003	1
Caelo	Carbomers	20003924004	11
Caelo	Carbomers	20003929003	2
Caelo	Carbomers	210000355001	1
Caelo	Carbomers	2100035001	1
Caelo	Carbomers	21000355001	13
Caelo	Carbomers	21000355004	6
Caelo	Carbomers	21000355006	1
Caelo	Carbomers	210003605008	1
Caelo	Carbomers	21001724001	6
Caelo	Carbomers	21001724002	13
Caelo	Carbomers	21001724004	3
Caelo	Carbomers	21001724008	3
Caelo	Carbomers	21001724009	2
Caelo	Carbomers	21002358004	2
Caelo	Carbomers	21003605001	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Carbomers	21003605003	8
Caelo	Carbomers	21003605008	9
Caelo	Carbomers	22002190003	7
Caelo	Carbomers	2215M-01232	1
Caelo	Carbomers	28111310	1
Caelo	Carbomers	2913M1232	1
Caelo	Carbomers	3000034003	1
Caelo	Carbomers	31631293	1
Caelo	Carbomers	3441	1
Caelo	Carbomers	42(20003924001)	1
Caelo	Carbomers	9011903	1
Caeol	Carbomers	16253004	1
Caesar & Loretz GmbH...	Carbomers	21001724008	1
Caesar & Loretz GmbH...	Carbomers	23000179002	1
Caesar & Loretz GmbH...	Carbomers	19227601	1
Caesar & Loretz GmbH...	Carbomers	21003605003	3
Caesar & Loretz GmbH...	Carbomers	19236601	1
Caesar & Loretz GmbH...	Carbomers	20000343003	1
Caesar & Loretz GmbH...	Carbomers	20003924004	1
Caesar & Loretz GmbH...	Carbomers	21001724002	1
Caesar & Loretz GmbH/Gehe	Carbomers	21001724001	1
Caesar & Loretz GmbH...	Carbomers	21001724001	1
Caesar & Loretz GmbH...	Carbomers	22002190003	1
Caesar & Loretz GmbH/Kehr	Carbomers	18307411	1
Caesar & Loretz GmbH/Kehr	Carbomers	20001190003	1
Caesar & Loretz GmbH/Kehr	Carbomers	21001724001	1
Caesar & Loretz GmbH...	Carbomers	19227601	1
Caesar & Loretz GmbH/L10	Carbomers	20001190003	1
Caesar & Loretz GmbH...	Carbomers	20003095003	1
Caesar & Loretz GmbH...	Carbomers	21001724008	1
Caesar & Loretz GmbH...	Carbomers	20003924004	1
Caesar & Loretz GmbH...	Carbomers	20003924004	2
Caesar & Loretz GmbH...	Carbomers	21000355001	1
Caesar & Loretz GmbH...	Carbomers	21000355004	1
Caesar & Loretz GmbH...	Carbomers	18307406	1
Caesar & Loretz GmbH...	Carbomers	18307410	1
Caesar & Loretz GmbH...	Carbomers	20003095003	1
Caesar & Loretz GmbH...	Carbomers	21000355001	1
Caesar & Loretz GmbH...	Carbomers	21003605008	1
Caesar & Loretz GmbH...	Carbomers	19227601	1
Caesar & Loretz GmbH...	Carbomers	21001724001	1
Caesar & Loretz GmbH...	Carbomers	19227602	1
Caesar & Loretz GmbH	Carbomers	18092401	2
Caesar & Loretz GmbH	Carbomers	18092405	1
Caesar & Loretz GmbH	Carbomers	18092406	1
Caesar & Loretz GmbH	Carbomers	18092408	1
Caesar & Loretz GmbH	Carbomers	18092412	1
Caesar & Loretz GmbH	Carbomers	18307401	1
Caesar & Loretz GmbH	Carbomers	18307402	1
Caesar & Loretz GmbH	Carbomers	18307406	2
Caesar & Loretz GmbH	Carbomers	18307407	3
Caesar & Loretz GmbH	Carbomers	18307408	1
Caesar & Loretz GmbH	Carbomers	18307410	3
Caesar & Loretz GmbH	Carbomers	18307411	2
Caesar & Loretz GmbH	Carbomers	19024501	1
Caesar & Loretz GmbH	Carbomers	19024505	1
Caesar & Loretz GmbH	Carbomers	1903007-01	1
Caesar & Loretz GmbH	Carbomers	192276004	4
Caesar & Loretz GmbH	Carbomers	192276005	1
Caesar & Loretz GmbH	Carbomers	19227602	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Carbomers	19227603	1
Caesar & Loretz GmbH	Carbomers	20000343001	2
Caesar & Loretz GmbH	Carbomers	20000343003	4
Caesar & Loretz GmbH	Carbomers	20001190003	7
Caesar & Loretz GmbH	Carbomers	20001190007	1
Caesar & Loretz GmbH	Carbomers	20001190008	2
Caesar & Loretz GmbH	Carbomers	20003095003	1
Caesar & Loretz GmbH	Carbomers	20003924001	6
Caesar & Loretz GmbH	Carbomers	20003924004	7
Caesar & Loretz GmbH	Carbomers	21000355001	1
Caesar & Loretz GmbH	Carbomers	21000355002	1
Caesar & Loretz GmbH	Carbomers	21000355004	6
Caesar & Loretz GmbH	Carbomers	21001724001	2
Caesar & Loretz GmbH	Carbomers	21001724002	2
Caesar & Loretz GmbH	Carbomers	21001724008	8
Caesar & Loretz GmbH	Carbomers	21003605001	2
Caesar & Loretz GmbH	Carbomers	21003605003	3
Caesar & Loretz GmbH	Carbomers	21003605008	3
Caesar & Loretz GmbH	Carbomers	22002070002	1
Caesar & Loretz GmbH	Carbomers	22002190003	4
Caesar & Loretz Hild...	Carbomers	18307403	1
Caesar & Loretz/Geil...	Carbomers	20000343003	1
Caesar & Loretz	Carbomers	18092408	1
Caesar & Loretz	Carbomers	18307408	1
Caesar&Loretz,Phönix...	Carbomers	15439003	1
Caesar/Phönix	Carbomers	21001724008	1
Cealo	Carbomers	18307408	1
Cordes/Phönix	Carbomers	192276004	1
Eu Rho	Carbomers	2203009-01	1
EuRho/ Noweda	Carbomers	1908029-01	1
EuRho/ Phönix	Carbomers	2003049-01	1
EuRho	Carbomers	1210037-01	1
EuRho	Carbomers	1311027-02	1
EuRho	Carbomers	1410001-01	2
Euro OTC	Carbomers		1
Euro OTC	Carbomers	101217279	1
Euro OTC	Carbomers	101616773	2
Euro OTC	Carbomers	102026590	1
Euro OTC	Carbomers	102540805	1
Euro OTC	Carbomers	120202001	2
Euro OTC	Carbomers	1202020-01	2
Euro OTC	Carbomers	12052014A	1
Euro OTC	Carbomers	1210037-01	6
Euro OTC	Carbomers	1305007-01	2
Euro OTC	Carbomers	130800601	1
Euro OTC	Carbomers	1311027-01	3
Euro OTC	Carbomers	1311027-02	7
Euro OTC	Carbomers	141000-01	1
Euro OTC	Carbomers	141000101	1
Euro OTC	Carbomers	1410001-01	13
Euro OTC	Carbomers	1512010-01	8
Euro OTC	Carbomers	1512010-02	5
Euro OTC	Carbomers	151210-02	1
Euro OTC	Carbomers	1518E2	1
Euro OTC	Carbomers	1604032-01	8
Euro OTC	Carbomers	1607028-01	10
Euro OTC	Carbomers	1610024-01	21
Euro OTC	Carbomers	16253002	1
Euro OTC	Carbomers	16253014	1
Euro OTC	Carbomers	1702012-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Carbomers	1706015-01	4
Euro OTC	Carbomers	17361402	1
Euro OTC	Carbomers	18010019-01	1
Euro OTC	Carbomers	1801044-01	6
Euro OTC	Carbomers	1810019-01	10
Euro OTC	Carbomers	18307401	1
Euro OTC	Carbomers	190300-01	1
Euro OTC	Carbomers	1903007-01	5
Euro OTC	Carbomers	1908029-01	3
Euro OTC	Carbomers	2003049-01	8
Euro OTC	Carbomers	210400701	1
Euro OTC	Carbomers	2104007-01	5
Euro OTC	Carbomers	2112003-01	1
Euro OTC	Carbomers	2203009-01	1
Euro OTC	Carbomers	2206008-01	4
Euro OTC	Carbomers	41(1810019-01)	1
Euro OTC	Carbomers	4311027-01	1
Euro/Gehe	Carbomers	1604032-01	1
Euro/Phönix	Carbomers	161002401	1
Euro/Sanacorp	Carbomers	1305007-01	1
Euro	Carbomers	1410001-01	2
Fagron	Carbomers	13194503	1
Fagron	Carbomers	1607028-01	1
Fiebig	Carbomers	2003049-01	1
Fischer/Gehe	Carbomers	1410001-02	1
Gatt-Koller	Carbomers	1800201	1
Gehe 04.11.21 EK:7,78EUR	Carbomers	211105CM	1
Gehe	Carbomers	102669851	1
Gehe	Carbomers	13194505	1
Gehe	Carbomers	16237501	1
GEHE	Carbomers	18092405	1
Gehe	Carbomers	18307408	1
Gehe	Carbomers	22002190003	1
Gehe	Carbomers	2302002-01	1
Hepart AG	Carbomers	12274916	1
Ichthyol/Phönix	Carbomers	14149905	1
Jenne	Carbomers	18049301	2
Kehr	Carbomers	23000685003	1
L10/apo-ident	Carbomers	1512010-01	1
L30	Carbomers	1610024-01	1
L30	Carbomers	1801044-01	2
Nachtestung	Carbomers		1
Noweda Taucha	Carbomers	21001724008	1
Noweda/ Caesar&Loren…	Carbomers	192276004	1
Noweda	Carbomers	16253012	1
Noweda	Carbomers	20000343003	1
Noweda	Carbomers	21000355004	1
Noweda	Carbomers	22002190003	1
Noweda	Carbomers	2206008-01	1
Noweda	Carbomers	23000823003	1
Pharbil Waltrop GmbH	Carbomers	102237289	4
Pharbil Waltrop GmbH	Carbomers	102246780	1
Phoenix 16.04.2014	Carbomers	13194503	1
Phoenix	Carbomers	18307402	1
Phoenix	Carbomers	19227602	1
Phoenix	Carbomers	20003924003	1
Phönix Gotha	Carbomers	19227601	1
Phönix	Carbomers	18092405	1
Phönix	Carbomers	18092411	1
Phönix	Carbomers	200011980008	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
PHÖNIX	Carbomers	21000355004	2
Phönix	Carbomers	22002190003	1
Rezepturlager - Verl…	Carbomers	115/14	1
Sanacaorp	Carbomers	14149905	1
Sanacorp	Carbomers	12274922	1
Sanacorp	Carbomers	1311027-01	1
Sanacorp	Carbomers	14149911	1
Sanacorp	Carbomers	1604032-01	1
Sanacorp	Carbomers	160702801	1
Sanacorp	Carbomers	18307411	1
Sanacorp	Carbomers	19227601	1
Sanacorp	Carbomers	20003924004	1
Sanacorp	Carbomers	20003929003	2
sanacorp	Carbomers	22002190002	1
Sanacorp	Carbomers	2302002-01	1
Sanacorp	Carbomers	6/AKD13	1

- 235 083 spectra from 1515 *Apo-Ident* customers from a total of 49 056 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Carbomers* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Carbomers* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	550	0	152 412
Type B	0	1040	0	201 044
Type C	0	982	2	235 083

The substance/substance group *Carbomers* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9091 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4231 %)
Type C	100.0000 % (> 99.9007 %)	99.7967 % (> 99.4919 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20978	20978	0.00	116.86
20979	20979	0.00	103.64
21354	22852	12.61	115.19
21557	22686	13.45	118.89
21561	22548	6.98	109.92
22250	22250	0.00	112.84
22548	22548	0.00	106.27
22686	22686	0.00	110.10
22759	22759	0.00	181.28
22852	22852	0.00	104.84
25809	25809	0.00	194.16
27218	27218	0.00	121.14

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Carmellose sodium**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20866-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Carmellose sodium; Carmellosum natricum

Special notes

When selecting the *Carmellose sodium* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Carmellose sodium	10	6	70

Second-stage model

For differentiation of the substance/substance group *Carmellose sodium* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Carmellose sodium* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	53.50	–
⋮	⋮	⋮
SyrSpend® SF Alka	>50	21.75
SyrSpend® SF pH4 neo (Maize starch)	>50	26.25
Colistin sulfate	>50	33.59
Calcium glycerophosphate	>50	38.38
Corn starch	>50	38.90
Rice starch	>50	39.18
Polymyxin B sulfate	65.97	39.41
Acacia, dried dispersion	>50	39.81
Amphotericin B	>50	45.90
Bacitracin	>50	46.57
Cyanocobalamin	>50	48.46
Wheat starch	>50	48.69
SyrSpend® SF pH4	>50	51.61
Selenium yeast	>50	64.72
Riboflavin	>50	66.20
Maltodextrin	>50	71.01
Potato starch	>50	74.59
Nystatin	>50	82.85
Tosylchloramide sodium	>50	89.37
Oxalic acid	>50	90.75
Calcium pantothenate	>50	101.23
alpha-tocopheryl acetate dry concentrate	>50	112.68
Gelatine, white	>50	113.39
Estradiol hemihydrate	>50	114.13
Hyoscine hydrobromide	>50	121.13
Estriol	>50	127.98
Triamcinolone	>50	149.47
Fructose	>50	176.93
Methylcobalamin	>50	195.43

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Carmellose sodium* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Carmellose sodium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Carmellose sodium	12354404	20866	40	1401185
Caelo	Carmellose sodium	13104807	20872	40	1401186
Caelo	Carmellose sodium	14029211	21382	40	20140127
Caelo	Carmellose sodium	13299310	21432	60	20131002
Caelo	Carmellose sodium	161714	22645	40	20160713*
Caelo	Carmellose sodium	16171406	23187	40	AR-17-FG-015964-01
Caelo	Carmellose sodium	180486	24039	40	20180228*
Caelo	Carmellose sodium	22002555	26352	40	20220922*
Caelo	Carmellose sodium	22002555	26352SI	20	20220922*
Fagron	Carmellose sodium	13D22-N02	20892	40	1401187
Fagron	Carmellose sodium	18E15-B04-354617	24868	40	20180620

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 440 spectra of 11 reference samples from the substance/substance group *Carmellose sodium*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.
- 152 522 spectra from a total of 2832 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 270 spectra of 8 reference samples from the substance/substance group *Carmellose sodium*.
- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Carmellose sodium	17062304	23519	40
Caelo	Carmellose sodium	172446	23623	40
Caelo	Carmellose sodium	20000171001	25500	40
Caelo	Carmellose sodium	22000132008	26311	30
Caelo	Carmellose sodium	23000402	26712	40
Caelo	Carmellose sodium	23001501	26844	40
Caelo	Carmellose sodium	22000132008	26311SI	20
Caelo	Carmellose sodium	23000402	26712SI	20

- 201 814 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 218 spectra from 132 *Apo-Ident* customers from 73 batches from the substance/substance group *Carmellose sodium*.
- Among them are spectra of independent samples from 70 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Carmellose sodium	22000132001	1
	Carmellose sodium	23000402001	2
	Carmellose sodium	23000402002	6
	Carmellose sodium	23000402005	4
	Carmellose sodium	23001501001	1
Bombastus	Carmellose sodium	13104813	1
Caelo	Carmellose sodium	10000620042	1
Caelo	Carmellose sodium	11124211	1
Caelo	Carmellose sodium	12255708	1
Caelo	Carmellose sodium	12354408	1
Caelo	Carmellose sodium	12354414	1
Caelo	Carmellose sodium	12354416	3
Caelo	Carmellose sodium	13104802	3
Caelo	Carmellose sodium	13104807	2
Caelo	Carmellose sodium	13104810	3
Caelo	Carmellose sodium	13104813	2
Caelo	Carmellose sodium	1315Q-03302	1
Caelo	Carmellose sodium	13299302	2
Caelo	Carmellose sodium	13G19-N02	1
Caelo	Carmellose sodium	14029201	1
Caelo	Carmellose sodium	14029211	1
Caelo	Carmellose sodium	14149806	2
Caelo	Carmellose sodium	15123901	5
Caelo	Carmellose sodium	15123908	5
Caelo	Carmellose sodium	15123909	1
Caelo	Carmellose sodium	15123912	1
Caelo	Carmellose sodium	16171402	3
Caelo	Carmellose sodium	17052304	1
Caelo	Carmellose sodium	17062303	2
Caelo	Carmellose sodium	17062304	4
Caelo	Carmellose sodium	17062307	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Carmellose sodium	17062308	2
Caelo	Carmellose sodium	17062309	3
Caelo	Carmellose sodium	17244601	2
Caelo	Carmellose sodium	17348601	8
Caelo	Carmellose sodium	17348604	1
Caelo	Carmellose sodium	17348605	7
Caelo	Carmellose sodium	17348606	1
Caelo	Carmellose sodium	180486003	8
Caelo	Carmellose sodium	18048602	2
Caelo	Carmellose sodium	18048604	13
Caelo	Carmellose sodium	18048607	1
Caelo	Carmellose sodium	2000132001	1
Caelo	Carmellose sodium	20001837002	5
Caelo	Carmellose sodium	21000062003	1
Caelo	Carmellose sodium	21000062004	6
Caelo	Carmellose sodium	21000062007	2
Caelo	Carmellose sodium	2119M-04170	1
Caelo	Carmellose sodium	218U-03302	1
Caelo	Carmellose sodium	22000132001	4
Caelo	Carmellose sodium	22000132002	2
Caelo	Carmellose sodium	22000132009	2
Caelo	Carmellose sodium	22002555003	2
Caelo	Carmellose sodium	22002555005	1
Caelo	Carmellose sodium	22002555006	2
Caelo	Carmellose sodium	22002555007	2
Caelo	Carmellose sodium	23000402002	5
Caelo	Carmellose sodium	23000402005	1
Caelo	Carmellose sodium	25041805	1
Caelo	Carmellose sodium	28051402	1
Caelo	Carmellose sodium	36/17	1
Caesar & Loretz GmbH…	Carmellose sodium	17244601	1
Caesar & Loretz GmbH…	Carmellose sodium	18048604	1
Caesar & Loretz GmbH…	Carmellose sodium	22002555007	1
Caesar & Loretz GmbH…	Carmellose sodium	18048604	1
Caesar & Loretz GmbH…	Carmellose sodium	20001837002	1
Caesar & Loretz GmbH…	Carmellose sodium	22002555006	1
Caesar & Loretz GmbH…	Carmellose sodium	18048604	1
Caesar & Loretz GmbH…	Carmellose sodium	18048604	3
Caesar & Loretz GmbH…	Carmellose sodium	23000402001	1
Caesar & Loretz GmbH	Carmellose sodium	17062307	1
Caesar & Loretz GmbH	Carmellose sodium	17348605	1
Caesar & Loretz GmbH	Carmellose sodium	18048604	1
Caesar & Loretz GmbH	Carmellose sodium	20001837002	5
Caesar & Loretz GmbH	Carmellose sodium	21000062004	3
Caesar & Loretz GmbH	Carmellose sodium	21000062007	1
Caesar & Loretz GmbH	Carmellose sodium	22000132001	1
Caesar & Loretz GmbH	Carmellose sodium	22000132002	1
Caesar & Loretz GmbH	Carmellose sodium	22000132009	2
Caesar & Loretz GmbH	Carmellose sodium	22002555003	1
Caesar & Loretz GmbH	Carmellose sodium	22002555006	2
Caesar & Loretz GmbH	Carmellose sodium	22002555007	1
Caesar & Loretz GmbH	Carmellose sodium	23000402002	3
Caesar & Loretz/AHD	Carmellose sodium	20001837002	1
Caesar&Loretz GmbH	Carmellose sodium	21000062007	1
Fagro	Carmellose sodium	15G03-B02-321790	1
Fagro	Carmellose sodium	16G05-B05-329314	1
Fagro	Carmellose sodium	17C20-B07-337104	1
Fagro	Carmellose sodium	17K06-B03-345975	1
Fagron	Carmellose sodium	13D22-N02	1
Fagron	Carmellose sodium	15G03-B02-312862	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Carmellose sodium	15G03-Bo2-312862	1
Fagron	Carmellose sodium	15G03-B02-321790	1
Fagron	Carmellose sodium	7006400006	1
Gehe 06.10.14	Carmellose sodium	13299312	1
Gehe	Carmellose sodium	17062307	1
GEHE	Carmellose sodium	17062307	1
Gehe	Carmellose sodium	22000132001	1
Gutenberg-Apotheke	Carmellose sodium	4811E-03302	1
Kehr	Carmellose sodium	22000132001	1
Kehr	Carmellose sodium	22002555003	1
Kehr	Carmellose sodium	2300402005	1
Noweda	Carmellose sodium	12354401	1
Noweda	Carmellose sodium	20001837002	1
Noweda	Carmellose sodium	22002555004	1
Phoenix	Carmellose sodium	17348601	2
Phönix	Carmellose sodium	23001501005	1
Sanacorp	Carmellose sodium	180486003	1
Sanacorp	Carmellose sodium	AKD6	1

- 235 849 spectra from 1515 *Apo-Ident* customers from a total of 49 188 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Carmellose sodium* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Carmellose sodium* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	270	0	201 814
Type C	0	217	1	235 849

The substance/substance group *Carmellose sodium* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.7778 %)
Type C	100.0000 % (> 99.9007 %)	99.5413 % (> 98.1651 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20866	20866	0.00	77.21
20872	20872	0.00	75.37
20892	20892	0.00	71.50
21382	20872	14.57	80.63
21432	20866	32.64	73.21
22645	22645	0.00	72.76
23187	23187	0.00	75.02
24039	24039	0.00	99.96
24868	20892	17.98	79.22
26352	26352	0.00	72.91

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cellulose, microcrystalline**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20708-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cellulose, microcrystalline; Cellulosum microcristallinum

Special notes

When selecting the *Cellulose, microcrystalline* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cellulose, microcrystalline	8	12	71

Second-stage model

For differentiation of the substance/substance group *Cellulose, microcrystalline* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cellulose, microcrystalline* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	75.87	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cellulose, microcrystalline* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cellulose, microcrystalline*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cellulose, microcrystalline	1201004-01	20728	40	20120201
Euro OTC	Cellulose, microcrystalline	1211037-01	21080	30	20121207
Euro OTC	Cellulose, microcrystalline	1211037-01	21085	40	20121207
Euro OTC	Cellulose, microcrystalline	1507022	21857	60	20150805*
Euro OTC	Cellulose, microcrystalline	1604029	22559	40	20160512*
Euro OTC	Cellulose, microcrystalline	2010026	25464	40	20201209*
Euro OTC	Cellulose, microcrystalline	2212016	26527	40	20230112*
Euro OTC	Cellulose, microcrystalline	2212016	26527SI	20	20230112*
Fagron	Cellulose, microcrystalline	12C23-N06	20708	70	1403080
Fagron	Cellulose, microcrystalline	16B24-B11-323324	22896	40	20160311

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 420 spectra of 10 reference samples from the substance/substance group *Cellulose, microcrystalline*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 542 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 540 spectra of 15 reference samples from the substance/substance group *Cellulose, microcrystalline*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Cellulose, microcrystalline	1607042	22794	40
Euro OTC	Cellulose, microcrystalline	1604029-01	22815	40
Euro OTC	Cellulose, microcrystalline	1610030	22876	40
Euro OTC	Cellulose, microcrystalline	1712009	23909	40
Euro OTC	Cellulose, microcrystalline	1811011	24346	40
Euro OTC	Cellulose, microcrystalline	1911018	25076	40
Euro OTC	Cellulose, microcrystalline	2005004	25248	40
Euro OTC	Cellulose, microcrystalline	2109026	25880	50
Euro OTC	Cellulose, microcrystalline	2309002	26938	40
Euro OTC	Cellulose, microcrystalline	2410009	27464	40
Fagron	Cellulose, microcrystalline	22A15-B01-217413	26293	40
Fagron	Cellulose, microcrystalline	24A09-B01-237270	27174	40
Euro OTC	Cellulose, microcrystalline	2109026	25880SI	10
Euro OTC	Cellulose, microcrystalline	2309002	26938SI	20
Fagron	Cellulose, microcrystalline	22A15-B01-217413	26293SI	20

- 201 544 spectra from a total of 4033 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 229 spectra from 152 *Apo-Ident* customers from 74 batches from the substance/substance group *Cellulose, microcrystalline*.

- Among them are spectra of independent samples from 71 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cellulose, microcrystalline	2010026-01	2
	Cellulose, microcrystalline	2109026-01	2
	Cellulose, microcrystalline	2212016-01	4
	Cellulose, microcrystalline	22K19-B10-224131	1
	Cellulose, microcrystalline	2309002-01	2
	Cellulose, microcrystalline	23L11-B04-235327	2
	Cellulose, microcrystalline	24A09-B01-237270	1
AHD	Cellulose, microcrystalline	2109026-1	1
Anzag	Cellulose, microcrystalline	2005004-01	1
apo-ident.	Cellulose, microcrystalline	1604029-01	1
apo-ident	Cellulose, microcrystalline	1610030-01	1
Caelo	Cellulose, microcrystalline	160402901	1
Caelo	Cellulose, microcrystalline	1610030-01	4
Caelo	Cellulose, microcrystalline	8722	1
DuPont	Cellulose, microcrystalline	R0025	1
EuRho	Cellulose, microcrystalline	1201004-02	1
Euro OTC	Cellulose, microcrystalline	1201004-02	2
Euro OTC	Cellulose, microcrystalline	121103701	1
Euro OTC	Cellulose, microcrystalline	1211037-01	2
Euro OTC	Cellulose, microcrystalline	1309001-01	3
Euro OTC	Cellulose, microcrystalline	1309001-02	3
Euro OTC	Cellulose, microcrystalline	135010001	1
Euro OTC	Cellulose, microcrystalline	1410002-01	5
Euro OTC	Cellulose, microcrystalline	1507022	1
Euro OTC	Cellulose, microcrystalline	150702201	1
Euro OTC	Cellulose, microcrystalline	150722-01	1
Euro OTC	Cellulose, microcrystalline	1604029-01	10
Euro OTC	Cellulose, microcrystalline	160704201	1
Euro OTC	Cellulose, microcrystalline	1607042-01	3
Euro OTC	Cellulose, microcrystalline	1610030-01	11
Euro OTC	Cellulose, microcrystalline	1704b50351755	1
Euro OTC	Cellulose, microcrystalline	1712009-01	2
Euro OTC	Cellulose, microcrystalline	1712009-02	7
Euro OTC	Cellulose, microcrystalline	1811011-01	18
Euro OTC	Cellulose, microcrystalline	181101103	1
Euro OTC	Cellulose, microcrystalline	1811011-03	6
Euro OTC	Cellulose, microcrystalline	1911018-01	6
Euro OTC	Cellulose, microcrystalline	195010861	2
Euro OTC	Cellulose, microcrystalline	2005004-01	10
Euro OTC	Cellulose, microcrystalline	201002601	2
Euro OTC	Cellulose, microcrystalline	2010026-01	31
Euro OTC	Cellulose, microcrystalline	205010638	3
Euro OTC	Cellulose, microcrystalline	2109026-01	7
Euro OTC	Cellulose, microcrystalline	2109026-02	3
Euro OTC	Cellulose, microcrystalline	2763	1
Euro OTC	Cellulose, microcrystalline	2780	1
Euro OTC	Cellulose, microcrystalline	7/21	1
Euro OTC	Cellulose, microcrystalline	700204	2
Euro OTC	Cellulose, microcrystalline	8710	1
Euro OTC	Cellulose, microcrystalline	SD17070102	2
Euro/Noweda	Cellulose, microcrystalline	1410002-02	1
Euro/Sanacorp	Cellulose, microcrystalline	1911018-01	1
Fagron	Cellulose, microcrystalline	13A03-N01	1
Fagron	Cellulose, microcrystalline	15C03-B06-305242	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cellulose, microcrystalline	17/04-B50	1
Fagron	Cellulose, microcrystalline	17/04-B50-351755	1
Fagron	Cellulose, microcrystalline	17A11-B04-331463	1
Fagron	Cellulose, microcrystalline	17A11-B04-340541	1
Fagron	Cellulose, microcrystalline	17I04-B50-351755	1
Fagron	Cellulose, microcrystalline	18/19-B50-360110	2
Fagron	Cellulose, microcrystalline	18B16-B50-355434	1
Fagron	Cellulose, microcrystalline	18K16-B50	1
Fagron	Cellulose, microcrystalline	18k16-b50-360224	1
Fagron	Cellulose, microcrystalline	18K16-B50-360224	1
Fagron	Cellulose, microcrystalline	18K16-B50-364001	1
Fagron	Cellulose, microcrystalline	18K16-B50-364002	1
Fagron	Cellulose, microcrystalline	18119-B05-360110	1
Fagron	Cellulose, microcrystalline	2005004-41	1
Fagron	Cellulose, microcrystalline	2013M-01350	1
Fagron	Cellulose, microcrystalline	205001122	1
Fagron	Cellulose, microcrystalline	20E15-F03-371624	1
Fagron	Cellulose, microcrystalline	20E15-F03-371625	1
Fagron	Cellulose, microcrystalline	20L01-F02	1
Fagron	Cellulose, microcrystalline	20L01-F02-376412	2
Fagron	Cellulose, microcrystalline	20L01F02376414	2
Fagron	Cellulose, microcrystalline	20L01-F02-376414	5
Fagron	Cellulose, microcrystalline	23C02-B11-226149	1
Fagron	Cellulose, microcrystalline	9K10-N10	1
Kehr	Cellulose, microcrystalline	2212016-01	1
Koisser	Cellulose, microcrystalline	E0790	1
Noweda	Cellulose, microcrystalline	1811011-03	1
Noweda	Cellulose, microcrystalline	1911018-01	1
Noweda	Cellulose, microcrystalline	2109026-01	1
Noweda	Cellulose, microcrystalline	2212016-01	1
Noweda	Cellulose, microcrystalline	2215016-01	1
Phnoix	Cellulose, microcrystalline	1211037-01	1
Phoenix	Cellulose, microcrystalline	1309001-02	1
Phoenix	Cellulose, microcrystalline	1712009-02	1
Phoenix	Cellulose, microcrystalline	3235	1
ROHA	Cellulose, microcrystalline	140010	1
Sanacorp/EuRho	Cellulose, microcrystalline	2109026-01	1
Sanacorp	Cellulose, microcrystalline	2005004-01	1
Sanacorp	Cellulose, microcrystalline	2010026-01	1
Sanacorp	Cellulose, microcrystalline	2212016-01	1

- 235 838 spectra from 1515 *Apo-Ident* customers from a total of 49 184 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cellulose, microcrystalline* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cellulose, microcrystalline* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	540	0	201 544
Type C	0	229	0	235 838

The substance/substance group *Cellulose, microcrystalline* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8889 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 97.3799 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20708	20708	0.00	119.62
20728	20708	9.57	121.37
21080	20708	8.74	118.71
21085	20708	8.43	119.61
21857	21857	0.00	115.20
22559	22559	0.00	117.57
22896	21857	7.63	116.00
25464	25464	0.00	118.42
26527	26527	0.00	112.93

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cetostearyl alcohol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20738-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cetostearyl alcohol; Alcohol cetylicus; Alcohol cetylicus et stearylicus; Alcohol cetylicus et stearylicus emulsificans A; Cetomacrogol emulsifying wax 1000 NI; Cetyl alcohol; Emulsifying cetostearyl alcohol (type A)

Special notes

When selecting the *Cetostearyl alcohol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cetostearyl alcohol	34	25	473

Second-stage model

For differentiation of the substance/substance group *Cetostearyl alcohol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cetostearyl alcohol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Non-ionic emulsifying alcohol	20.37	–
Glycerol monostearate, emulsifying	42.62	–
Glycerol monostearate 60	69.82	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cetostearyl alcohol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cetostearyl alcohol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cetomacrogol emulsifying …	14055001	21381	40	20140225
Caelo	Cetomacrogol emulsifying …	15277504	22390	40	20150828
Caelo	Cetomacrogol emulsifying …	20000858003	25519	40	20200330
Caelo	Cetomacrogol emulsifying …	21002092004	25978	35	2208569
Caelo	Cetomacrogol emulsifying …	22002953003	26744	40	20221012
Caelo	Cetomacrogol emulsifying …	22002953003	26744SI	20	20221012
Fagron	Cetomacrogol emulsifying …	12H07-N06	20738	40	20120905
Fagron	Cetomacrogol emulsifying …	13C05-B40-289262	21054	40	1408003
Caelo	Cetostearyl alcohol	14054504	21314	40	20140226
Caelo	Cetostearyl alcohol	14054504	21442	60	20140226
Caelo	Cetostearyl alcohol	17049205	23725	40	20170302
Caelo	Cetostearyl alcohol	20002898002	25499	40	20200916
Caelo	Cetostearyl alcohol	21003928003	26231	40	20211208
Caelo	Cetostearyl alcohol	23000403	26698	40	20230228*
Caelo	Cetostearyl alcohol	23002042	26941	40	20230922*
Caelo	Cetostearyl alcohol	23002042	26941SI	20	20230922*
Fagron	Cetostearyl alcohol	13C13-N13	20968	40	1402265
Caelo	Cetyl alcohol	13096901	20896	40	1405179
Caelo	Cetyl alcohol	13286502	21318	40	20130925
Caelo	Cetyl alcohol	13286502	21435	60	20130925

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cetyl alcohol	15323301	22266	60	AR-16-FG-008835-01
Caelo	Cetyl alcohol	161063	22398	40	20160420*
Caelo	Cetyl alcohol	161063	22399	40	20160420*
Caelo	Cetyl alcohol	161063	22400	40	20160420*
Caelo	Cetyl alcohol	161063	22401	40	20160420*
Caelo	Cetyl alcohol	161063	22402	40	20160420*
Caelo	Cetyl alcohol	161063	22403	40	20160420*
Caelo	Cetyl alcohol	20002637001	25498	40	20201009
Caelo	Cetyl alcohol	22000377002	26586	40	20220308
Caelo	Cetyl alcohol	22000377002	26586SI	20	20220308
Caelo	Cetyl alcohol	23000249	26695	40	20230224*
Caelo	Cetyl alcohol	23000249	26695SI	20	20230224*
Caelo	Cetyl alcohol	23000130	26697	40	20230224*
Caelo	Cetyl alcohol	23000130	26697SI	20	20230224*
Euro OTC	Cetyl alcohol	1508014-01	22611	40	20150821
Bombastus	Emulsifying cetostearyl a…	21004319	26025	40	20211011
Caelo	Emulsifying cetostearyl a…	13233005	21319	30	1506057
Caelo	Emulsifying cetostearyl a…	13233005	21434	60	20130816
Caelo	Emulsifying cetostearyl a…	14322505	21830	60	20141031
Caelo	Emulsifying cetostearyl a…	153857	22331	60	20151202*
Caelo	Emulsifying cetostearyl a…	153857	22332	60	20151202*
Caelo	Emulsifying cetostearyl a…	153856	22333	60	20160210*
Caelo	Emulsifying cetostearyl a…	153856	22334	60	20160210*
Euro OTC	Emulsifying cetostearyl a…	1510043	21998	60	20151124*
Euro OTC	Emulsifying cetostearyl a…	1504010-01	22264	60	20150423
Euro OTC	Emulsifying cetostearyl a…	2002033	25253	40	20200617*
Euro OTC	Emulsifying cetostearyl a…	2012002	25528	40	20210104*
Fagron	Emulsifying cetostearyl a…	13L17-B05	21279	40	1505070
Fagron	Emulsifying cetostearyl a…	16I13-B01-326511	23022	40	20161024

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 2065 spectra of 49 reference samples from the substance/substance group *Cetostearyl alcohol*. These samples are listed above in the *calibration samples* section. The reference samples come from 34 different batches.
- 150 897 spectra from a total of 2808 batches from further 480 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Type B spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1260 spectra of 34 reference samples from the substance/substance group *Cetostearyl alcohol*.
- Among them are spectra of independent samples from 25 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cetomacrogol emulsifying …	160804	22395	40
Caelo	Cetostearyl alcohol	170492	23097	40
Caelo	Cetostearyl alcohol	172979	23819	40
Caelo	Cetostearyl alcohol	190552	24721	40
Caelo	Cetostearyl alcohol	21000059005	25935	40
Caelo	Cetostearyl alcohol	24001586	27328	40
Caelo	Cetyl alcohol	170473	23068	40
Caelo	Cetyl alcohol	173155	23973	40
Caelo	Cetyl alcohol	21001593	25697	50
Caelo	Cetyl alcohol	23003036	27420	40
Caelo	Cetyl alcohol	24002178	27421	40
Bombastus	Emulsifying cetostearyl a…	23004942	27060	40
Caelo	Emulsifying cetostearyl a…	171980	23575	40
Caelo	Emulsifying cetostearyl a…	180180	24033	40
Caelo	Emulsifying cetostearyl a…	191857	25068	40
Caelo	Emulsifying cetostearyl a…	20002023	25377	40
Caelo	Emulsifying cetostearyl a…	21000566	25663	40
Caelo	Emulsifying cetostearyl a…	22004149	26699	40
Caelo	Emulsifying cetostearyl a…	24002417	27417	40
Euro OTC	Emulsifying cetostearyl a…	1604013	22540	40
Euro OTC	Emulsifying cetostearyl a…	1701031	22999	40
Euro OTC	Emulsifying cetostearyl a…	1705001	23381	40
Euro OTC	Emulsifying cetostearyl a…	1711001	23737	40
Fagron	Emulsifying cetostearyl a…	23A11-B07-224497	26611	40
Fagron	Emulsifying cetostearyl a…	24G09-B04-003936	27470	40
Caelo	Cetomacrogol emulsifying …	160804	22396	40
Caelo	Cetomacrogol emulsifying …	160804	22397	40
Caelo	Cetomacrogol emulsifying …	21002092004	25978SI†	30
Caelo	Cetostearyl alcohol	21003928003	26231SI†	20
Caelo	Cetostearyl alcohol	23000403	26698SI†	20
Bombastus	Emulsifying cetostearyl a…	23004942	27060SI	20
Caelo	Emulsifying cetostearyl a…	22004149	26699SI	20
Euro OTC	Emulsifying cetostearyl a…	1711001	25093	40
Fagron	Emulsifying cetostearyl a…	23A11-B07-224497	26611SI	20

- 200 824 spectra from a total of 4017 batches from further 835 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1599 spectra from 607 *Apo-Ident* customers from 402 batches from the substance/substance group *Cetostearyl alcohol*.
- Among them are spectra of independent samples from 381 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cetostearyl alcohol	1711001-02	1
	Emulsifying cetostearyl a...	2012002-02	1
	Cetostearyl alcohol	21000086001	2
	Emulsifying cetostearyl a...	21003223011	3
	Cetyl alcohol	22000377002	1
	Cetomacrogol emulsifying ...	22001170001	2
	Emulsifying cetostearyl a...	22001324007	1
	Emulsifying cetostearyl a...	22001329004	4
	Emulsifying cetostearyl a...	22001329007	1
	Emulsifying cetostearyl a...	22001329008	10
	Cetostearyl alcohol	22003074003	1
	Emulsifying cetostearyl a...	22004149004	2
	Emulsifying cetostearyl a...	2201329008	1
	Emulsifying cetostearyl a...	22C11-B02-222108	1
	Cetyl alcohol	23000130003	1
	Cetyl alcohol	23000130004	6
	Cetyl alcohol	2300013004	1
	Cetyl alcohol	23003036008	1
	Emulsifying cetostearyl a...	23A11-B07-224497	1
	Cetyl alcohol	23E25-B05_230388	1
	Cetyl alcohol	522202021	1
A.H.D.	Emulsifying cetostearyl a...	12L19-N03	2
ahd/lamotte	Cetostearyl alcohol	13210504	1
AHD	Cetyl alcohol	17321603	1
AHD	Cetyl alcohol	20002637001	1
AHD	Cetomacrogol emulsifying ...	8073743	1
ALH	Emulsifying cetostearyl a...	15271405	1
Alliance Health 24.0...	Emulsifying cetostearyl a...	13L17-B05-289805	1
alliance health. 05....	Emulsifying cetostearyl a...	14G31-B03-297610	1
Anzag	Emulsifying cetostearyl a...	12G02-N04	1
Audor Pharma	Emulsifying cetostearyl a...	16238602	1
BASF / Sanacorp	Emulsifying cetostearyl a...	B04-1953003	1
Bombastus	Emulsifying cetostearyl a...	18000081P-180824-1	1
Bombastus	Emulsifying cetostearyl a...	18000081P181203-4	1
Bombastus	Emulsifying cetostearyl a...	18000081P-190312-9	1
Bombastus	Emulsifying cetostearyl a...	18002312	3
Bombastus	Emulsifying cetostearyl a...	18003404	1
Bombastus	Emulsifying cetostearyl a...	18003437	4
Bombastus	Emulsifying cetostearyl a...	18006205P-190312-10	1
Bombastus	Emulsifying cetostearyl a...	19002555	5
Bombastus	Emulsifying cetostearyl a...	19005207P-200116-3	1
Bombastus	Emulsifying cetostearyl a...	19005208	2
Bombastus	Emulsifying cetostearyl a...	20001742	1
Bombastus	Emulsifying cetostearyl a...	20005694	2
Bombastus	Emulsifying cetostearyl a...	265360	1
Bombastus	Emulsifying cetostearyl a...	278418	1
Bombastus	Emulsifying cetostearyl a...	288691	3
Bombastus	Emulsifying cetostearyl a...	295148	2
Bombastus	Emulsifying cetostearyl a...	300132	5
Bombastus	Emulsifying cetostearyl a...	303935	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Emulsifying cetostearyl a…	308514	5
Bombastus	Emulsifying cetostearyl a…	60083112P-200326-4	1
Caelo	Emulsifying cetostearyl a…		3
Caelo	Emulsifying cetostearyl a…	11009204	1
Caelo	Cetyl alcohol	1112013B	1
Caelo	Cetyl alcohol	11153405	1
Caelo	Cetostearyl alcohol	11162305	1
Caelo	Emulsifying cetostearyl a…	11291101	1
Caelo	Emulsifying cetostearyl a…	11291103	1
Caelo	Cetostearyl alcohol	11302101	1
Caelo	Cetyl alcohol	11320702	2
Caelo	Cetyl alcohol	12018605	2
Caelo	Cetostearyl alcohol	12021304	1
Caelo	Cetostearyl alcohol	12025301	2
Caelo	Emulsifying cetostearyl a…	12065709	7
Caelo	Cetyl alcohol	1212E-01076	1
Caelo	Emulsifying cetostearyl a…	12134203	1
Caelo	Emulsifying cetostearyl a…	12229402	2
Caelo	Emulsifying cetostearyl a…	12231402	1
Caelo	Cetyl alcohol	12271103	5
Caelo	Emulsifying cetostearyl a…	12331402	7
Caelo	Emulsifying cetostearyl a…	12331407	3
Caelo	Cetyl alcohol	12338604	6
Caelo	Emulsifying cetostearyl a…	12C30-N01	1
Caelo	Cetostearyl alcohol	13018305	4
Caelo	Cetostearyl alcohol	13018306	1
Caelo	Cetyl alcohol	13096901	5
Caelo	Cetyl alcohol	13096904	2
Caelo	Cetostearyl alcohol	1314405	1
Caelo	Emulsifying cetostearyl a…	13144103	1
Caelo	Emulsifying cetostearyl a…	13144104	2
Caelo	Emulsifying cetostearyl a…	13144105	12
Caelo	Emulsifying cetostearyl a…	13144107	2
Caelo	Cetostearyl alcohol	13206206	3
Caelo	Cetyl alcohol	13210504	9
Caelo	Emulsifying cetostearyl a…	13233001	1
Caelo	Emulsifying cetostearyl a…	13233002	3
Caelo	Emulsifying cetostearyl a…	13233005	12
Caelo	Emulsifying cetostearyl a…	13233006	1
Caelo	Emulsifying cetostearyl a…	13233008	2
Caelo	Cetyl alcohol	13286502	5
Caelo	Emulsifying cetostearyl a…	13352102	1
Caelo	Cetostearyl alcohol	13-B01-327355	1
Caelo	Emulsifying cetostearyl a…	13L17-B05-289806	1
Caelo	Cetostearyl alcohol	14054504	4
Caelo	Cetostearyl alcohol	14054508	3
Caelo	Cetomacrogol emulsifying …	14055002	1
Caelo	Cetostearyl alcohol	14061317	1
Caelo	Emulsifying cetostearyl a…	14156201	1
Caelo	Emulsifying cetostearyl a…	14158201	13
Caelo	Emulsifying cetostearyl a…	14158202	1
Caelo	Cetostearyl alcohol	14215007	6
Caelo	Cetyl alcohol	14262204	5
Caelo	Emulsifying cetostearyl a…	14322502	2
Caelo	Emulsifying cetostearyl a…	14322505	12
Caelo	Emulsifying cetostearyl a…	14322506	2
Caelo	Emulsifying cetostearyl a…	14322512	1
Caelo	Cetostearyl alcohol	14346201	3
Caelo	Cetostearyl alcohol	14346202	1
Caelo	Cetyl alcohol	14349101	14

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Emulsifying cetostearyl a…	14G31-B03-305612	3
Caelo	Emulsifying cetostearyl a…	15071704	1
Caelo	Emulsifying cetostearyl a…	15090701	10
Caelo	Emulsifying cetostearyl a…	15090703	2
Caelo	Emulsifying cetostearyl a…	15090706	3
Caelo	Emulsifying cetostearyl a…	1510043-01	1
Caelo	Cetomacrogol emulsifying …	15113703	1
Caelo	Cetyl alcohol	1523316	1
Caelo	Emulsifying cetostearyl a…	15271402	9
Caelo	Emulsifying cetostearyl a…	15271403	9
Caelo	Emulsifying cetostearyl a…	15271405	12
Caelo	Emulsifying cetostearyl a…	15271407	9
Caelo	Emulsifying cetostearyl a…	15271408	3
Caelo	Emulsifying cetostearyl a…	15271410	1
Caelo	Cetostearyl alcohol	15272702	2
Caelo	Cetostearyl alcohol	15272709	6
Caelo	Cetostearyl alcohol	15272717	6
Caelo	Cetomacrogol emulsifying …	15277501	1
Caelo	Cetomacrogol emulsifying …	15277505	1
Caelo	Cetyl alcohol	15323301	7
Caelo	Cetyl alcohol	15323308	1
Caelo	Cetyl alcohol	15323311	11
Caelo	Cetyl alcohol	15323316	4
Caelo	Emulsifying cetostearyl a…	15385602	3
Caelo	Emulsifying cetostearyl a…	15385606	1
Caelo	Emulsifying cetostearyl a…	15789271	1
Caelo	Emulsifying cetostearyl a…	15C31-B99-307062	1
Caelo	Cetostearyl alcohol	16048812	3
Caelo	Cetomacrogol emulsifying …	16080403	1
Caelo	Cetomacrogol emulsifying …	16080407	2
Caelo	Cetostearyl alcohol	160914	1
Caelo	Cetyl alcohol	16106307	4
Caelo	Emulsifying cetostearyl a…	16119604	14
Caelo	Emulsifying cetostearyl a…	16119607	2
Caelo	Cetostearyl alcohol	16230603	2
Caelo	Emulsifying cetostearyl a…	16238604	3
Caelo	Emulsifying cetostearyl a…	16238607	11
Caelo	Cetyl alcohol	16335802	7
Caelo	Cetyl alcohol	16335805	1
Caelo	Cetyl alcohol	16335807	7
Caelo	Cetomacrogol emulsifying …	16348101	2
Caelo	Emulsifying cetostearyl a…	16I13-B01-327355	1
Caelo	Emulsifying cetostearyl a…	16I13-B01-327864	1
Caelo	Cetyl alcohol	17047303	1
Caelo	Cetyl alcohol	17047306	3
Caelo	Cetyl alcohol	17047307	13
Caelo	Cetostearyl alcohol	17049209	2
Caelo	Cetostearyl alcohol	1705001-01	1
Caelo	Emulsifying cetostearyl a…	17056802	1
Caelo	Emulsifying cetostearyl a…	17056806	6
Caelo	Cetostearyl alcohol	1711001-02	2
Caelo	Cetostearyl alcohol	171215CSA/15272717	1
Caelo	Emulsifying cetostearyl a…	17132001	11
Caelo	Emulsifying cetostearyl a…	17139201	5
Caelo	Emulsifying cetostearyl a…	17198002	5
Caelo	Emulsifying cetostearyl a…	17198003	24
Caelo	Cetomacrogol emulsifying …	17210402	1
Caelo	Cetyl alcohol	17234902	1
Caelo	Cetyl alcohol	17234903	1
Caelo	Cetyl alcohol	17234904	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Emulsifying cetostearyl a…	17261701	2
Caelo	Emulsifying cetostearyl a…	17261702	4
Caelo	Cetostearyl alcohol	17321303	9
Caelo	Cetostearyl alcohol	17321305	1
Caelo	Cetostearyl alcohol	17321319	1
Caelo	Cetostearyl alcohol	17321603	16
Caelo	Cetyl alcohol	17321612	6
Caelo	Cetostearyl alcohol	17D28-B06-334609	1
Caelo	Emulsifying cetostearyl a…	17D28-B06-338141	2
Caelo	Emulsifying cetostearyl a…	17F21-B01-341021	1
Caelo	Emulsifying cetostearyl a…	18003401	1
Caelo	Emulsifying cetostearyl a…	18003404	13
Caelo	Emulsifying cetostearyl a…	18006205P-190719-1	1
Caelo	Emulsifying cetostearyl a…	18018001	4
Caelo	Emulsifying cetostearyl a…	18018002	1
Caelo	Emulsifying cetostearyl a…	18018003P-190308-2	1
Caelo	Emulsifying cetostearyl a…	18018005	9
Caelo	Emulsifying cetostearyl a…	18018006	2
Caelo	Emulsifying cetostearyl a…	18081201	1
Caelo	Cetyl alcohol	18153102	17
Caelo	Cetyl alcohol	18237701	19
Caelo	Cetostearyl alcohol	18248502	12
Caelo	Cetostearyl alcohol	18248510	3
Caelo	Emulsifying cetostearyl a…	18291403	2
Caelo	Emulsifying cetostearyl a…	18291404	16
Caelo	Emulsifying cetostearyl a…	18291406	4
Caelo	Emulsifying cetostearyl a…	18291407	10
Caelo	Emulsifying cetostearyl a…	18291408	1
Caelo	Cetostearyl alcohol	18A23-B04	1
Caelo	Emulsifying cetostearyl a…	18A23-B04-349155	1
Caelo	Cetostearyl alcohol	18A23-B04-352987	2
Caelo	Emulsifying cetostearyl a…	19005207P-191101-2	1
Caelo	Cetyl alcohol	19012504	6
Caelo	Cetyl alcohol	19012509	11
Caelo	Emulsifying cetostearyl a…	19032014B	1
Caelo	Emulsifying cetostearyl a…	19055206	5
Caelo	Emulsifying cetostearyl a…	191857002	23
Caelo	Emulsifying cetostearyl a…	19185702	24
Caelo	Emulsifying cetostearyl a…	19185703	3
Caelo	Cetostearyl alcohol	192139002	3
Caelo	Cetostearyl alcohol	192139007	3
Caelo	Cetomacrogol emulsifying …	192199001	2
Caelo	Cetyl alcohol	192219005	16
Caelo	Emulsifying cetostearyl a…	192747003	9
Caelo	Emulsifying cetostearyl a…	192747007	27
Caelo	Cetyl alcohol	192921001	9
Caelo	Cetyl alcohol	200002637001	1
Caelo	Cetomacrogol emulsifying …	20000858003	3
Caelo	Cetomacrogol emulsifying …	20002050001	1
Caelo	Cetyl alcohol	20002637001	18
Caelo	Cetostearyl alcohol	20002898002	5
Caelo	Cetyl alcohol	20004011001	1
Caelo	Cetyl alcohol	2002637001	1
Caelo	Emulsifying cetostearyl a…	2011404	1
Caelo	Cetyl alcohol	20250112-1	1
Caelo	Emulsifying cetostearyl a…	20F30B01200749	1
Caelo	Emulsifying cetostearyl a…	210000566007	1
Caelo	Cetostearyl alcohol	21000059001	9
Caelo	Cetostearyl alcohol	21000059005	8
Caelo	Emulsifying cetostearyl a…	21000086001	23

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Emulsifying cetostearyl a…	21000086002	5
Caelo	Emulsifying cetostearyl a…	21000086003	1
Caelo	Cetyl alcohol	210001593001	1
Caelo	Emulsifying cetostearyl a…	21000566	1
Caelo	Emulsifying cetostearyl a…	21000566005	1
Caelo	Emulsifying cetostearyl a…	21000566006	1
Caelo	Emulsifying cetostearyl a…	21000566007	13
Caelo	Cetostearyl alcohol	2100059001	1
Caelo	Emulsifying cetostearyl a…	2100086001	2
Caelo	Cetostearyl alcohol	21001071005	1
Caelo	Emulsifying cetostearyl a…	21001071007	5
Caelo	Cetyl alcohol	21001593001	11
Caelo	Cetomacrogol emulsifying …	21002092002	2
Caelo	Cetomacrogol emulsifying …	21002092004	2
Caelo	Cetyl alcohol	21002870003	5
Caelo	Emulsifying cetostearyl a…	21003223003	9
Caelo	Emulsifying cetostearyl a…	21003223008	5
Caelo	Emulsifying cetostearyl a…	21003223010	2
Caelo	Cetostearyl alcohol	21003928003	3
Caelo	Cetostearyl alcohol	22001324007	3
Caelo	Emulsifying cetostearyl a…	22001329004	2
Caelo	Cetostearyl alcohol	2201324007	1
Caelo	Emulsifying cetostearyl a…	23051503	1
Caelo	Emulsifying cetostearyl a…	23091402	1
Caelo	Emulsifying cetostearyl a…	24101305	1
Caelo	Emulsifying cetostearyl a…	25/AKD1	1
Caelo	Emulsifying cetostearyl a…	25051201	1
Caelo	Cetyl alcohol	28101701	1
Caelo	Emulsifying cetostearyl a…	29091803	1
Caelo	Emulsifying cetostearyl a…	303935	1
Caelo	Emulsifying cetostearyl a…	31032015B	1
Caelo	Emulsifying cetostearyl a…	3256	1
Caelo	Emulsifying cetostearyl a…	5011505	1
Caelo	Emulsifying cetostearyl a…	608/10072017	1
Caelo	Cetyl alcohol	7071807	1
Caelo	Cetostearyl alcohol	8041708	1
Caelo	Emulsifying cetostearyl a…	9170717	1
Caelo	Emulsifying cetostearyl a…	Unbekannt	1
Caeolo	Emulsifying cetostearyl a…	17056807	1
Caesar & Lorenz GmbH	Emulsifying cetostearyl a…	18291404	1
Caesar & Loretz GmbH…	Emulsifying cetostearyl a…	21003223003	1
Caesar & Loretz GmbH…	Emulsifying cetostearyl a…	18018005	1
Caesar & Loretz GmbH…	Cetyl alcohol	22000377002	1
Caesar & Loretz GmbH…	Cetostearyl alcohol	11302101	1
Caesar & Loretz GmbH…	Emulsifying cetostearyl a…	192747005	1
Caesar & Loretz GmbH…	Cetyl alcohol	21001593001	2
Caesar & Loretz GmbH…	Emulsifying cetostearyl a…	191857002	4
Caesar & Loretz GmbH…	Cetyl alcohol	20002637001	1
Caesar & Loretz GmbH…	Cetostearyl alcohol	21000059001	1
Caesar & Loretz GmbH…	Emulsifying cetostearyl a…	21000086001	2
Caesar & Loretz GmbH…	Emulsifying cetostearyl a…	192747007	1
Caesar & Loretz GmbH…	Emulsifying cetostearyl a…	21000566007	1
Caesar & Loretz GmbH/Gehe	Emulsifying cetostearyl a…	18291401	1
Caesar & Loretz GmbH/Gehe	Cetyl alcohol	20002637001	1
Caesar & Loretz GmbH/Gehe	Emulsifying cetostearyl a…	21000566006	1
Caesar & Loretz GmbH…	Cetostearyl alcohol	21001071007	1
Caesar & Loretz GmbH…	Cetostearyl alcohol	22001324007	1
Caesar & Loretz GmbH…	Emulsifying cetostearyl a…	18291404	1
Caesar & Loretz GmbH…	Emulsifying cetostearyl a…	191857002	1
Caesar & Loretz GmbH…	Emulsifying cetostearyl a…	21000086001	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Cetostearyl alcohol	19055206	1
Caesar & Loretz GmbH...	Cetostearyl alcohol	19185702	1
Caesar & Loretz GmbH...	Cetostearyl alcohol	21001071007	1
Caesar & Loretz GmbH...	Emulsifying cetostearyl a...	21003223008	1
Caesar & Loretz GmbH...	Emulsifying cetostearyl a...	21003223010	1
Caesar & Loretz GmbH...	Cetyl alcohol	19012509	1
Caesar & Loretz GmbH...	Emulsifying cetostearyl a...	19185702	1
Caesar & Loretz GmbH...	Emulsifying cetostearyl a...	21000566007	1
Caesar & Loretz GmbH...	Emulsifying cetostearyl a...	21001071007	1
Caesar & Loretz GmbH/Sana	Cetyl alcohol	192219005	2
Caesar & Loretz GmbH...	Cetostearyl alcohol	18291404	2
Caesar & Loretz GmbH...	Emulsifying cetostearyl a...	18291406	1
Caesar & Loretz GmbH...	Emulsifying cetostearyl a...	21000566007	1
Caesar & Loretz GmbH...	Cetyl alcohol	21001593001	1
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	13233008	1
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	16119604	3
Caesar & Loretz GmbH	Cetostearyl alcohol	17056806	1
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	17132001	1
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	18018005	1
Caesar & Loretz GmbH	Cetomacrogol emulsifying ...	18143802	1
Caesar & Loretz GmbH	Cetyl alcohol	18153102	3
Caesar & Loretz GmbH	Cetyl alcohol	18237701	3
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	18248502	5
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	18291403	2
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	18291404	2
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	18291407	1
Caesar & Loretz GmbH	Cetyl alcohol	19012504	2
Caesar & Loretz GmbH	Cetyl alcohol	19012509	2
Caesar & Loretz GmbH	Cetostearyl alcohol	19055206	3
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	191857002	5
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	19185702	6
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	19185704	1
Caesar & Loretz GmbH	Cetostearyl alcohol	192139002	3
Caesar & Loretz GmbH	Cetostearyl alcohol	192139007	3
Caesar & Loretz GmbH	Cetomacrogol emulsifying ...	192199001	1
Caesar & Loretz GmbH	Cetyl alcohol	192219005	4
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	192747005	1
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	192747007	9
Caesar & Loretz GmbH	Cetostearyl alcohol	192921001	3
Caesar & Loretz GmbH	Cetomacrogol emulsifying ...	20000858003	1
Caesar & Loretz GmbH	Cetyl alcohol	20001279002	1
Caesar & Loretz GmbH	Cetomacrogol emulsifying ...	20002050001	2
Caesar & Loretz GmbH	Cetyl alcohol	20002637001	7
Caesar & Loretz GmbH	Cetostearyl alcohol	20002898002	2
Caesar & Loretz GmbH	Cetostearyl alcohol	21000059001	3
Caesar & Loretz GmbH	Cetyl alcohol	21000059005	1
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	21000086001	7
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	21000086003	2
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	21000566007	4
Caesar & Loretz GmbH	Cetostearyl alcohol	21001071007	1
Caesar & Loretz GmbH	Cetyl alcohol	21001593001	2
Caesar & Loretz GmbH	Cetyl alcohol	21002870003	2
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	21003223002	2
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	21003223003	1
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	21003223010	1
Caesar & Loretz GmbH	Cetostearyl alcohol	21003928003	1
Caesar & Loretz GmbH	Cetyl alcohol	22000377001	1
Caesar & Loretz GmbH	Cetostearyl alcohol	22001324007	1
Caesar & Loretz GmbH	Emulsifying cetostearyl a...	22001329004	3
Caesar & Loretz GmbH	Cetostearyl alcohol	22003074003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz/Gehe	Cetyl alcohol	19012504	1
Caesar & Loretz/Geil...	Emulsifying cetostearyl a...	192747007	1
Caesar & Loretz	Emulsifying cetostearyl a...	18291407	1
Caesar & Noweda	Emulsifying cetostearyl a...	19185703	1
Caesar &Loretz GmbH	Emulsifying cetostearyl a...	12065703	1
Caesar&loretz,Phoenix	Emulsifying cetostearyl a...	14158201	1
Caesar&Loretz/Noweda	Emulsifying cetostearyl a...	15271405	1
Caesar/Lorenz	Emulsifying cetostearyl a...	13233005	1
Caesar/Noweda	Emulsifying cetostearyl a...	11343405	1
Caesar/Noweda	Emulsifying cetostearyl a...	12065707	1
Caesar/Noweda	Cetostearyl alcohol	15272705	1
Caesar/Noweda	Cetostearyl alcohol	2911E-01077	2
Calo/AHD	Cetyl alcohol	192921001	1
Cealo/AHD	Cetostearyl alcohol	16106307	1
Cealo/Alliance Healthcare	Cetostearyl alcohol	18291403	1
Cealo/Sanacorp	Cetostearyl alcohol	21003223003	1
Cealo	Cetostearyl alcohol	15385602	2
Cealo	Cetostearyl alcohol	19012504	1
Celo/Jenne	Emulsifying cetostearyl a...	21000086001	1
Ebert-Jacobi	Cetostearyl alcohol	16230603	1
EuRho Anzag ek:3,47EUR	Cetyl alcohol	110505501	1
EuRho	Cetyl alcohol	1206020-01	1
Euro OTC	Emulsifying cetostearyl a...	10836573	1
Euro OTC	Cetyl alcohol	1105055-01	1
Euro OTC	Cetostearyl alcohol	1107035-01	1
Euro OTC	Cetostearyl alcohol	1204015-01	1
Euro OTC	Cetyl alcohol	1206020-01	1
Euro OTC	Cetyl alcohol	1211002-01	2
Euro OTC	Emulsifying cetostearyl a...	1212019-01	1
Euro OTC	Emulsifying cetostearyl a...	1305035-01	2
Euro OTC	Emulsifying cetostearyl a...	1404019-01	2
Euro OTC	Emulsifying cetostearyl a...	1404019-02	2
Euro OTC	Emulsifying cetostearyl a...	1404019-03	1
Euro OTC	Emulsifying cetostearyl a...	14G31-B03-297610	1
Euro OTC	Cetostearyl alcohol	150401001	1
Euro OTC	Emulsifying cetostearyl a...	1504010-01	3
Euro OTC	Emulsifying cetostearyl a...	150410-01	1
Euro OTC	Cetyl alcohol	1508014-01	1
Euro OTC	Cetyl alcohol	150818C	1
Euro OTC	Emulsifying cetostearyl a...	1510043-01	4
Euro OTC	Emulsifying cetostearyl a...	15271403	2
Euro OTC	Emulsifying cetostearyl a...	1604013-02	5
Euro OTC	Emulsifying cetostearyl a...	1701031-01	5
Euro OTC	Cetostearyl alcohol	17050001-01	1
Euro OTC	Emulsifying cetostearyl a...	1705001-01	11
Euro OTC	Emulsifying cetostearyl a...	171001-02	1
Euro OTC	Emulsifying cetostearyl a...	1711001-02	5
Euro OTC	Emulsifying cetostearyl a...	17110011-01	1
Euro OTC	Cetyl alcohol	18153102	1
Euro OTC	Emulsifying cetostearyl a...	2002033-01	3
Euro OTC	Emulsifying cetostearyl a...	2012002-01	1
Euro OTC	Cetostearyl alcohol	2012002-02	1
Euro OTC	Cetostearyl alcohol	20270912-2	1
Euro OTC	Emulsifying cetostearyl a...	21897043	1
Euro OTC	Cetostearyl alcohol	2806	1
Euro/Gehe	Emulsifying cetostearyl a...	150401-01	1
Euroh/Noweda	Emulsifying cetostearyl a...	1504010-01	1
Fagro	Emulsifying cetostearyl a...	5211Q-01078	1
Fagron	Cetostearyl alcohol	10F17-N02	1
Fagron	Emulsifying cetostearyl a...	11499002	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cetostearyl alcohol	11E17-N13	1
Fagron	Cetostearyl alcohol	11f30-n11	1
Fagron	Emulsifying cetostearyl a…	11L22-N09	1
Fagron	Cetostearyl alcohol	12/17-N05	1
Fagron	Emulsifying cetostearyl a…	12602-N04	1
Fagron	Cetyl alcohol	12A-02N12	1
Fagron	Emulsifying cetostearyl a…	12C30-N01	2
Fagron	Cetostearyl alcohol	12E30-N13	1
Fagron	Cetostearyl alcohol	12g02-n04	1
Fagron	Emulsifying cetostearyl a…	12G02N04	1
Fagron	Emulsifying cetostearyl a…	12G02-N04	12
Fagron	Cetostearyl alcohol	12J17-N05	2
Fagron	Cetostearyl alcohol	12J17-NO5	1
Fagron	Emulsifying cetostearyl a…	12J29-N04	4
Fagron	Cetostearyl alcohol	12K22-N03	3
Fagron	Emulsifying cetostearyl a…	12L19-N03	8
Fagron	Cetostearyl alcohol	13C13-N13	1
Fagron	Emulsifying cetostearyl a…	13F07-N05	9
Fagron	Emulsifying cetostearyl a…	13I06-N04	1
Fagron	Emulsifying cetostearyl a…	13L17-B05	2
Fagron	Emulsifying cetostearyl a…	13L17B05289805	1
Fagron	Emulsifying cetostearyl a…	13L17-B05-289805	7
Fagron	Emulsifying cetostearyl a…	13L17-B05-289806	5
Fagron	Emulsifying cetostearyl a…	13L17-B05-289807	1
Fagron	Emulsifying cetostearyl a…	13L17-B05-294999	4
Fagron	Cetostearyl alcohol	14346201	1
Fagron	Emulsifying cetostearyl a…	14G31-B03	1
Fagron	Emulsifying cetostearyl a…	14G31-B03-297610	2
Fagron	Cetostearyl alcohol	14G31-B03-297611	1
Fagron	Emulsifying cetostearyl a…	14G31-B03-305612	4
Fagron	Emulsifying cetostearyl a…	15789271	2
Fagron	Emulsifying cetostearyl a…	15C31-B00-307062	1
Fagron	Emulsifying cetostearyl a…	15C31-B99-307062	5
Fagron	Emulsifying cetostearyl a…	15D24-B02	2
Fagron	Emulsifying cetostearyl a…	15D24-B02-308261	5
Fagron	Emulsifying cetostearyl a…	15D24-B02-311993	9
Fagron	Emulsifying cetostearyl a…	16/13-B01-327355	2
Fagron	Emulsifying cetostearyl a…	16/13-B01-331290	1
Fagron	Emulsifying cetostearyl a…	16/13-Bo1-327864	1
Fagron	Emulsifying cetostearyl a…	161006CSA	1
Fagron	Emulsifying cetostearyl a…	16990201	1
Fagron	Emulsifying cetostearyl a…	16B23-B07	1
Fagron	Emulsifying cetostearyl a…	16B23-B07-318218	4
Fagron	Emulsifying cetostearyl a…	16B23-B07-320384	7
Fagron	Emulsifying cetostearyl a…	16B23-B07-323025	3
Fagron	Emulsifying cetostearyl a…	16I13-B01	2
Fagron	Emulsifying cetostearyl a…	16I13-B01_326511	1
Fagron	Emulsifying cetostearyl a…	17028-B06-334609	1
Fagron	Emulsifying cetostearyl a…	171216CAE/0016830715	1
Fagron	Cetyl alcohol	17321612	1
Fagron	Emulsifying cetostearyl a…	17894959	1
Fagron	Emulsifying cetostearyl a…	17D21-B01-341021	1
Fagron	Emulsifying cetostearyl a…	17D28-B06	2
Fagron	Emulsifying cetostearyl a…	17D28-B06-334609	6
Fagron	Emulsifying cetostearyl a…	17D28-B06-338141	8
Fagron	Cetostearyl alcohol	17F21-B01	1
Fagron	Emulsifying cetostearyl a…	17F21-B01-341021	10
Fagron	Emulsifying cetostearyl a…	17F21-B01-344775	3
Fagron	Emulsifying cetostearyl a…	18003401	1
Fagron	Emulsifying cetostearyl a…	18A12-B04-355659	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cetostearyl alcohol	18A23-B04	1
Fagron	Emulsifying cetostearyl a…	18A23-B04-349155	8
Fagron	Emulsifying cetostearyl a…	18A23-B04-352987	6
Fagron	Emulsifying cetostearyl a…	18A23-B04-355659	2
Fagron	Cetostearyl alcohol	18A23-B64	1
Fagron	Emulsifying cetostearyl a…	19/04-B04-195303	1
Fagron	Emulsifying cetostearyl a…	19104-B04-195303	2
Fagron	Emulsifying cetostearyl a…	19I04-B04	1
Fagron	Emulsifying cetostearyl a…	19I04-B04-195303	5
Fagron	Cetostearyl alcohol	19I04-BO4-195303	1
Fagron	Emulsifying cetostearyl a…	19IO4-BO4-195303	2
Fagron	Cetostearyl alcohol	19l04-B04-195303	1
Fagron	Emulsifying cetostearyl a…	20260712-2	1
Fagron	Emulsifying cetostearyl a…	20F30B01200749	1
Fagron	Emulsifying cetostearyl a…	20F30-B01-200749	8
Fagron	Emulsifying cetostearyl a…	21139741	1
Fagron	Emulsifying cetostearyl a…	21J20-B05-213671	3
Fagron	Emulsifying cetostearyl a…	2215I-01078	1
Fagron	Emulsifying cetostearyl a…	22803390	1
Fagron	Emulsifying cetostearyl a…	22C11-B02-222108	1
Fagron	Emulsifying cetostearyl a…	2717M-01078	1
Fagron	Emulsifying cetostearyl a…	2797	1
Fagron	Emulsifying cetostearyl a…	2918E-01078	1
Fagron	Emulsifying cetostearyl a…	297611	1
Fagron	Emulsifying cetostearyl a…	3013M-01078	1
Fagron	Cetostearyl alcohol	3414E-01078	1
Fagron	Emulsifying cetostearyl a…	68955-20-4	1
Fagron	Cetostearyl alcohol	7886542	1
Fagron	Emulsifying cetostearyl a…	8256792	4
Fagron	Emulsifying cetostearyl a…	9652865	2
Fagron	Emulsifying cetostearyl a…	B04-1953003	1
fargon	Emulsifying cetostearyl a…	18A23-B04-352987	1
Fiebig	Cetostearyl alcohol	21000059001	1
Finze	Cetyl alcohol	10321703	1
fragron	Emulsifying cetostearyl a…	16l13-b01-326511	1
Gatt-Koller	Cetyl alcohol	1690/06162416	1
Gatt-Koller	Cetostearyl alcohol	1803965	1
Gehe	Emulsifying cetostearyl a…	12L19-N03	1
Gehe	Cetostearyl alcohol	15272713	1
Gehe	Cetostearyl alcohol	15272717	1
Gehe	Emulsifying cetostearyl a…	1701031-01	1
Gehe	Cetyl alcohol	18237701	1
Gehe	Emulsifying cetostearyl a…	18291406	1
Gehe	Cetyl alcohol	19012504	1
Gehe	Emulsifying cetostearyl a…	22001329004	1
GEHE	Emulsifying cetostearyl a…	22001329908	1
Gehe	Emulsifying cetostearyl a…	22004149004	1
Gehe	Emulsifying cetostearyl a…	22004189	1
Gepepharm/Gehe	Cetyl alcohol	181531102	1
Henry Lamotte / Noweda	Emulsifying cetostearyl a…	300132	1
Herba	Cetostearyl alcohol	KNC1133J18	1
Kehr	Cetyl alcohol	17047303	1
Kehr	Emulsifying cetostearyl a…	18003404	1
Kehr	Emulsifying cetostearyl a…	22001329004	2
Klenk	Emulsifying cetostearyl a…	16238607	1
Krieger	Emulsifying cetostearyl a…	1711001-01	1
Krieger	Cetyl alcohol	19012509	1
L12	Emulsifying cetostearyl a…	17056806	1
Nachprüfung	Emulsifying cetostearyl a…	123456	2
Noweda/ Caesar&Loren…	Cetyl alcohol	192921001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Cetostearyl alcohol	12065709	1
Noweda	Emulsifying cetostearyl a…	13065576	1
Noweda	Emulsifying cetostearyl a…	13144104	1
Noweda	Emulsifying cetostearyl a…	13CA9	1
Noweda	Cetostearyl alcohol	17321303	1
Noweda	Emulsifying cetostearyl a…	18003404	1
Noweda	Emulsifying cetostearyl a…	18018005	1
Noweda	Cetostearyl alcohol	18248510	1
Noweda	Emulsifying cetostearyl a…	192747007	1
Noweda	Emulsifying cetostearyl a…	22001329008	2
Noweda	Cetomacrogol emulsifying …	22002953003	2
Pala	Emulsifying cetostearyl a…	19185702	1
Ph.Eur/AHD	Cetostearyl alcohol	18291407	1
Phoenix 10.01.2020	Cetyl alcohol	19012509	1
Phoenix 26.11.12	Emulsifying cetostearyl a…	13144105	1
PHOENIX am07.04.2014	Emulsifying cetostearyl a…	13F07-N05	1
Phoenix	Cetostearyl alcohol	14322505	1
Phoenix	Emulsifying cetostearyl a…	15789271	1
Phoenix	Emulsifying cetostearyl a…	17198003	1
Phoenix	Emulsifying cetostearyl a…	17D28-B06-338141	1
Phoenix	Cetomacrogol emulsifying …	18335402	1
Phoenix	Cetostearyl alcohol	18A23-B04-352987	1
Phoenix	Cetostearyl alcohol	192139007	1
Phoenix	Emulsifying cetostearyl a…	21003223010	1
Phoenix	Cetostearyl alcohol	3071	1
Phönix, Caesar&Loret…	Emulsifying cetostearyl a…	192747007	1
Phönix	Cetyl alcohol	13096901	1
Phonix	Cetyl alcohol	13210504	1
Phönix	Emulsifying cetostearyl a…	1323305	1
Phönix	Emulsifying cetostearyl a…	15C31-B99-307062	1
Phönix	Cetostearyl alcohol	17D28-B06-338141	1
Phönix	Emulsifying cetostearyl a…	18A23-B04-355659	1
Phönix	Emulsifying cetostearyl a…	191857002	1
Phönix	Emulsifying cetostearyl a…	19185702	1
Phönix	Emulsifying cetostearyl a…	20005694	1
Phönix	Emulsifying cetostearyl a…	21000566007	3
Phönix	Emulsifying cetostearyl a…	22001329008	1
Phönx	Emulsifying cetostearyl a…	210086001	1
Sanacorp/Bombstus	Emulsifying cetostearyl a…	18003437	2
Sanacorp	Emulsifying cetostearyl a…	12J29-N04	1
Sanacorp	Cetostearyl alcohol	13206206	1
Sanacorp	Emulsifying cetostearyl a…	13F07-N05	4
Sanacorp	Emulsifying cetostearyl a…	13I06-N04	1
Sanacorp	Emulsifying cetostearyl a…	15090701	1
Sanacorp	Emulsifying cetostearyl a…	17198003	1
Sanacorp	Cetyl alcohol	17321603	1
Sanacorp	Emulsifying cetostearyl a…	191857002	1
Sanacorp	Emulsifying cetostearyl a…	210032230058	1
Sanacorp	Emulsifying cetostearyl a…	21003223011	2
Sanacorp	Cetostearyl alcohol	22003074003	1
Sanacorp	Cetostearyl alcohol	575778	1
Sanacorpaelo /Sanacorp	Cetyl alcohol	1AKS11	1
Spinnrad/ Noweda/ 19…	Cetyl alcohol	219302021	1
Spinnrad/Sanacorp	Cetyl alcohol	1018202022	1
Spinnrad	Cetyl alcohol	115202022	1
Spinnrad	Cetyl alcohol	416202023	1
Spinnrad	Cetyl alcohol	418302021	1
spinrad/pHÖNIX	Cetyl alcohol	418202021	1
Taoasis	Emulsifying cetostearyl a…	303935	2

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 234 468 spectra from 1515 *Apo-Ident* customers from a total of 48 862 batches from a further 718 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cetostearyl alcohol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cetostearyl alcohol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	2065	0	150 897
Type B	0	1260	0	200 824
Type C	0	1595	4	234 468

The substance/substance group *Cetostearyl alcohol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.7094 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.5238 %)
Type C	100.0000 % (> 99.9007 %)	99.7498 % (> 99.5622 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20738	21054	7.42	80.12
20896	20896	0.00	128.52
20968	20968	0.00	132.51
21054	21054	0.00	75.39
21279	21279	0.00	135.00
21314	26698	21.65	128.73
21318	20896	50.16	127.68
21319	21319	0.00	125.14
21381	21998	17.95	86.62
21434	22334	3.89	134.97

continued on the next page

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21435	20896	49.97	126.88
21442	26698	14.63	130.04
21830	21998	3.37	102.21
21998	21998	0.00	114.65
22264	22334	3.46	135.55
22266	22266	0.00	129.51
22331	22331	0.00	129.37
22332	22332	0.00	143.48
22333	22333	0.00	122.59
22334	22334	0.00	135.13
22390	21054	9.70	88.16
22398	22398	0.00	129.71
22399	22399	0.00	129.43
22400	22400	0.00	128.89
22401	22401	0.00	128.69
22402	22402	0.00	128.23
22403	22403	0.00	132.29
22611	22401	27.08	123.94
23022	22334	3.45	136.84
23725	26698	15.07	131.87
25253	25253	0.00	93.08
25498	26695	11.76	133.67
25499	21998	27.05	130.21
25519	21054	10.12	88.11
25528	25528	0.00	132.26
25978	25978	0.00	35.03
26025	22333	8.99	109.37
26231	26698	11.90	132.18
26586	26695	6.51	132.49
26695	26695	0.00	132.11
26697	26697	0.00	129.39
26698	26698	0.00	133.19
26744	21054	10.75	89.18
26941	26941	0.00	132.52

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Chloral hydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20322-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Chloral hydrate; Chlorali hydras

Special notes

When selecting the *Chloral hydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Chloral hydrate	6	11	189

Second-stage model

For differentiation of the substance/substance group *Chloral hydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Chloral hydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	91.99	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Chloral hydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Chloral hydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Chloral hydrate	13213311	21309	40	20130712
Caelo	Chloral hydrate	15448318	22963	40	1704462
Caelo	Chloral hydrate	16355802	23094	40	20170112
Fagron	Chloral hydrate	13F06-N07	21231	40	20130626
Fagron	Chloral hydrate	17E05-B05-335580	23572	40	20170623
Fagron	Chloral hydrate	19K04-B01-201434	25488	40	20191128

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 6 reference samples from the substance/substance group *Chloral hydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.
- 152 722 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 530 spectra of 14 reference samples from the substance/substance group *Chloral hydrate*.
- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Chloral hydrate	154483	23355	40
Caelo	Chloral hydrate	172506	23646	40
Caelo	Chloral hydrate	172477	23678	40
Caelo	Chloral hydrate	190914	24556	40
Caelo	Chloral hydrate	192361	24882	40
Caelo	Chloral hydrate	192872	24891	40
Caelo	Chloral hydrate	21001025	25668	50
Caelo	Chloral hydrate	22004038	26689	40
Caelo	Chloral hydrate	24001050	27304	40
Fagron	Chloral hydrate	22D25-B01-220429	26180	40
Fagron	Chloral hydrate	24A24-B10-238074	27185	40
Caelo	Chloral hydrate	172477	23815	40
Caelo	Chloral hydrate	22004038	26689SI	20
Fagron	Chloral hydrate	22D25-B01-220429	26180SI	20

- 201 554 spectra from a total of 4034 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1091 spectra from 423 *Apo-Ident* customers from 195 batches from the substance/substance group *Chloral hydrate*.
- Among them are spectra of independent samples from 189 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Chloral hydrate	10224/2311B066	1
	Chloral hydrate	21001025007	1
	Chloral hydrate	21001025014	1
	Chloral hydrate	21001025019	1
	Chloral hydrate	21001025020	3
	Chloral hydrate	21001025024	2
	Chloral hydrate	22004038001	12
	Chloral hydrate	22004038003	1
	Chloral hydrate	22004038004	5
	Chloral hydrate	22004038007	3
	Chloral hydrate	2204038001	1
	Chloral hydrate	24002447003	1
	Chloral hydrate	24A24-B10-001840	1
	Chloral hydrate	24A24-B10-229467	2
	Chloral hydrate	B08-0018309	1
AHD	Chloral hydrate	22004038001	1
Anzag	Chloral hydrate	20003841003	1
Apotheke Tellingstedt	Chloral hydrate	19091404	1
Bombastus	Chloral hydrate	17346301	1
Caelo	Chloral hydrate		1
Caelo	Chloral hydrate	1(2002323002)	1
Caelo	Chloral hydrate	12017503	1
Caelo	Chloral hydrate	12017512	1
Caelo	Chloral hydrate	12017518	1
Caelo	Chloral hydrate	13002425	2
Caelo	Chloral hydrate	13213311	1
Caelo	Chloral hydrate	13d22-n11	1
Caelo	Chloral hydrate	1403815	1
Caelo	Chloral hydrate	14038301	2
Caelo	Chloral hydrate	14038306	1
Caelo	Chloral hydrate	14038311	5
Caelo	Chloral hydrate	14101307	1
Caelo	Chloral hydrate	14218701	1
Caelo	Chloral hydrate	14218704	3
Caelo	Chloral hydrate	14218705	3
Caelo	Chloral hydrate	14218709	5
Caelo	Chloral hydrate	14218710	1
Caelo	Chloral hydrate	14218711	1
Caelo	Chloral hydrate	14218712	1
Caelo	Chloral hydrate	14218713	2
Caelo	Chloral hydrate	14218714	4
Caelo	Chloral hydrate	14218719	4
Caelo	Chloral hydrate	14218720	1
Caelo	Chloral hydrate	15083701	2
Caelo	Chloral hydrate	15083703	8
Caelo	Chloral hydrate	15083704	1
Caelo	Chloral hydrate	15083705	2
Caelo	Chloral hydrate	15163901	1
Caelo	Chloral hydrate	15166501	4
Caelo	Chloral hydrate	15166502	3
Caelo	Chloral hydrate	15166503	4
Caelo	Chloral hydrate	15166505	11
Caelo	Chloral hydrate	15166506	7
Caelo	Chloral hydrate	15166507	10
Caelo	Chloral hydrate	15166508	6
Caelo	Chloral hydrate	15166513	3
Caelo	Chloral hydrate	15448303	3
Caelo	Chloral hydrate	15448304	2
Caelo	Chloral hydrate	15448306	7
Caelo	Chloral hydrate	15448307	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Chloral hydrate	15448310	1
Caelo	Chloral hydrate	15448312	11
Caelo	Chloral hydrate	15448313	8
Caelo	Chloral hydrate	15448314	6
Caelo	Chloral hydrate	15448315	6
Caelo	Chloral hydrate	15448318	10
Caelo	Chloral hydrate	15448320	6
Caelo	Chloral hydrate	15448321	7
Caelo	Chloral hydrate	15448322	7
Caelo	Chloral hydrate	15448324	10
Caelo	Chloral hydrate	15448325	2
Caelo	Chloral hydrate	15448326	10
Caelo	Chloral hydrate	15448327	1
Caelo	Chloral hydrate	15458322	1
Caelo	Chloral hydrate	160906C	1
Caelo	Chloral hydrate	16248703	1
Caelo	Chloral hydrate	16355803	1
Caelo	Chloral hydrate	16355804	2
Caelo	Chloral hydrate	16355810	1
Caelo	Chloral hydrate	16355811	2
Caelo	Chloral hydrate	17121402	1
Caelo	Chloral hydrate	17247702	20
Caelo	Chloral hydrate	17247704	16
Caelo	Chloral hydrate	17250601	14
Caelo	Chloral hydrate	17314301	3
Caelo	Chloral hydrate	17314303	1
Caelo	Chloral hydrate	17314309	1
Caelo	Chloral hydrate	17314312	1
Caelo	Chloral hydrate	17314318	2
Caelo	Chloral hydrate	17314319	1
Caelo	Chloral hydrate	17314320	1
Caelo	Chloral hydrate	17314322	5
Caelo	Chloral hydrate	173406306	1
Caelo	Chloral hydrate	1734602	1
Caelo	Chloral hydrate	17346301	28
Caelo	Chloral hydrate	17346302	16
Caelo	Chloral hydrate	173463021	1
Caelo	Chloral hydrate	17346303	5
Caelo	Chloral hydrate	17346306	45
Caelo	Chloral hydrate	17346307	21
Caelo	Chloral hydrate	17346308	14
Caelo	Chloral hydrate	17346309	11
Caelo	Chloral hydrate	17346310	12
Caelo	Chloral hydrate	17346311	10
Caelo	Chloral hydrate	1746302	1
Caelo	Chloral hydrate	17520601	1
Caelo	Chloral hydrate	17550601	1
Caelo	Chloral hydrate	18054001	1
Caelo	Chloral hydrate	18327909	1
Caelo	Chloral hydrate	19000511001	12
Caelo	Chloral hydrate	19000511003	5
Caelo	Chloral hydrate	19091401	6
Caelo	Chloral hydrate	19091402	1
Caelo	Chloral hydrate	19091404	5
Caelo	Chloral hydrate	19091405	4
Caelo	Chloral hydrate	19091408	4
Caelo	Chloral hydrate	19091409	3
Caelo	Chloral hydrate	19091410	3
Caelo	Chloral hydrate	19236101	12
Caelo	Chloral hydrate	19236102	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Chloral hydrate	19236103	2
Caelo	Chloral hydrate	19236104	3
Caelo	Chloral hydrate	192872001	37
Caelo	Chloral hydrate	192872002	3
Caelo	Chloral hydrate	192872003	4
Caelo	Chloral hydrate	192872004	3
Caelo	Chloral hydrate	19287201	8
Caelo	Chloral hydrate	19287206	5
Caelo	Chloral hydrate	200002323002	1
Caelo	Chloral hydrate	20002323002	35
Caelo	Chloral hydrate	20002323004	6
Caelo	Chloral hydrate	2000233002	1
Caelo	Chloral hydrate	20003841002	11
Caelo	Chloral hydrate	20003841003	42
Caelo	Chloral hydrate	20003841005	2
Caelo	Chloral hydrate	2003841003	1
Caelo	Chloral hydrate	2019Q-01257	1
Caelo	Chloral hydrate	21001025002	6
Caelo	Chloral hydrate	21001025003	4
Caelo	Chloral hydrate	21001025004	29
Caelo	Chloral hydrate	21001025005	19
Caelo	Chloral hydrate	21001025007	4
Caelo	Chloral hydrate	21001025009	1
Caelo	Chloral hydrate	21001025010	15
Caelo	Chloral hydrate	21001025014	1
Caelo	Chloral hydrate	21001025015	5
Caelo	Chloral hydrate	21001025016	1
Caelo	Chloral hydrate	21001025017	4
Caelo	Chloral hydrate	21001025019	1
Caelo	Chloral hydrate	21001025020	1
Caelo	Chloral hydrate	21001025023	1
Caelo	Chloral hydrate	210010250236	2
Caelo	Chloral hydrate	21001025024	6
Caelo	Chloral hydrate	2100105004	1
Caelo	Chloral hydrate	22004038001	1
Caelo	Chloral hydrate	25021401	1
Caelo	Chloral hydrate	2818A-01257	1
Caelo	Chloral hydrate	2826	1
Caelo	Chloral hydrate	30081807	1
Caelo	Chloral hydrate	3121403	1
Caelo	Chloral hydrate	3299	1
Caelo	Chloral hydrate	3333	1
Caelo	Chloral hydrate	3449	1
Caelo	Chloral hydrate	4616Q-01257	1
Caelo	Chloral hydrate	6051703	1
Caelo	Chloral hydrate	928720011	1
Caeol/Noweda	Chloral hydrate	15448313	1
Caesar & Lorenz GmbH	Chloral hydrate	19000511001	1
Caesar & Lorenz GmbH	Chloral hydrate	192872001	1
Caesar & Loretz GmbH...	Chloral hydrate	20003841003	1
Caesar & Loretz GmbH...	Chloral hydrate	21001025004	1
Caesar & Loretz GmbH...	Chloral hydrate	21001025004	1
Caesar & Loretz GmbH...	Chloral hydrate	21001025005	1
Caesar & Loretz GmbH...	Chloral hydrate	20003841003	1
Caesar & Loretz GmbH...	Chloral hydrate	20003841003	2
Caesar & Loretz GmbH...	Chloral hydrate	119236101	1
Caesar & Loretz GmbH...	Chloral hydrate	20002323002	1
Caesar & Loretz GmbH/Gehe	Chloral hydrate	19000511001	1
Caesar & Loretz GmbH/Gehe	Chloral hydrate	19236101	1
Caesar & Loretz GmbH/Gehe	Chloral hydrate	20002323002	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Gehe	Chloral hydrate	20003841003	1
Caesar & Loretz GmbH/Gehe	Chloral hydrate	21001025005	1
Caesar & Loretz GmbH/Gehe	Chloral hydrate	21001025020	3
Caesar & Loretz GmbH/Gehe	Chloral hydrate	21001025024	1
Caesar & Loretz GmbH...	Chloral hydrate	20002323003	2
Caesar & Loretz GmbH...	Chloral hydrate	19287206	1
Caesar & Loretz GmbH...	Chloral hydrate	20002323002	2
Caesar & Loretz GmbH...	Chloral hydrate	20003841003	1
Caesar & Loretz GmbH...	Chloral hydrate	21001025010	1
Caesar & Loretz GmbH...	Chloral hydrate	21001025016	1
Caesar & Loretz GmbH...	Chloral hydrate	21001025024	2
Caesar & Loretz GmbH...	Chloral hydrate	22004038001	4
Caesar & Loretz GmbH...	Chloral hydrate	192872001	1
Caesar & Loretz GmbH...	Chloral hydrate	21001025010	1
Caesar & Loretz GmbH...	Chloral hydrate	21001025024	1
Caesar & Loretz GmbH	Chloral hydrate	17314317	1
Caesar & Loretz GmbH	Chloral hydrate	17314319	2
Caesar & Loretz GmbH	Chloral hydrate	17314320	1
Caesar & Loretz GmbH	Chloral hydrate	17346301	1
Caesar & Loretz GmbH	Chloral hydrate	17346310	1
Caesar & Loretz GmbH	Chloral hydrate	19000511001	3
Caesar & Loretz GmbH	Chloral hydrate	19091401	1
Caesar & Loretz GmbH	Chloral hydrate	19091409	2
Caesar & Loretz GmbH	Chloral hydrate	19236101	1
Caesar & Loretz GmbH	Chloral hydrate	19236104	1
Caesar & Loretz GmbH	Chloral hydrate	192872001	6
Caesar & Loretz GmbH	Chloral hydrate	192872002	1
Caesar & Loretz GmbH	Chloral hydrate	192872004	3
Caesar & Loretz GmbH	Chloral hydrate	19287201	1
Caesar & Loretz GmbH	Chloral hydrate	19287206	1
Caesar & Loretz GmbH	Chloral hydrate	20002323002	11
Caesar & Loretz GmbH	Chloral hydrate	20002323004	6
Caesar & Loretz GmbH	Chloral hydrate	20002323022	1
Caesar & Loretz GmbH	Chloral hydrate	20003841002	6
Caesar & Loretz GmbH	Chloral hydrate	20003841003	13
Caesar & Loretz GmbH	Chloral hydrate	20003841004	2
Caesar & Loretz GmbH	Chloral hydrate	20003841005	3
Caesar & Loretz GmbH	Chloral hydrate	21001025002	2
Caesar & Loretz GmbH	Chloral hydrate	21001025003	1
Caesar & Loretz GmbH	Chloral hydrate	21001025004	5
Caesar & Loretz GmbH	Chloral hydrate	21001025005	3
Caesar & Loretz GmbH	Chloral hydrate	21001025007	1
Caesar & Loretz GmbH	Chloral hydrate	21001025009	2
Caesar & Loretz GmbH	Chloral hydrate	21001025010	10
Caesar & Loretz GmbH	Chloral hydrate	21001025012	2
Caesar & Loretz GmbH	Chloral hydrate	21001025016	3
Caesar & Loretz GmbH	Chloral hydrate	21001025017	1
Caesar & Loretz GmbH	Chloral hydrate	21001025024	1
Caesar & Loretz GmbH	Chloral hydrate	21001025026	1
Caesar & Loretz Hild...	Chloral hydrate	192872001	1
Caesar & Loretz/AHD	Chloral hydrate	20002323002	1
Caesar & Loretz/Noweda	Chloral hydrate	20003841003	1
Caesar/Phoenix	Chloral hydrate	17250601	1
Caesar	Chloral hydrate	15166501	1
Cealo/ Alliance	Chloral hydrate	17247702	1
chaelo/gehe	Chloral hydrate	20003841003	3
Chemische Fabrik Ber...	Chloral hydrate	192872001	2
Ebert & Jacobi	Chloral hydrate	16D14-B02-322991	1
Ebert KKH 10.10.16	Chloral hydrate	15448308	1
Eder Apotheke	Chloral hydrate	19236101	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Chloral hydrate	15448318	1
Euro OTC	Chloral hydrate	16122001	1
Fagron	Chloral hydrate	11D13-N07	1
Fagron	Chloral hydrate	11J05-N01	1
Fagron	Chloral hydrate	12C26-M04	1
Fagron	Chloral hydrate	12C26-M05	1
Fagron	Chloral hydrate	12H06_N08	1
Fagron	Chloral hydrate	12H06N08	2
Fagron	Chloral hydrate	12H06-N08	6
Fagron	Chloral hydrate	12H06-N080101/1612	1
Fagron	Chloral hydrate	12H06-N080160/161	1
Fagron	Chloral hydrate	12H06N8	1
Fagron	Chloral hydrate	13D22-N11	1
Fagron	Chloral hydrate	13F06-N07	2
Fagron	Chloral hydrate	13F06-N070631/786	1
Fagron	Chloral hydrate	13K05-B13	1
Fagron	Chloral hydrate	14218710	1
Fagron	Chloral hydrate	14218712	1
Fagron	Chloral hydrate	15166505	1
Fagron	Chloral hydrate	160609/1	1
Fagron	Chloral hydrate	17346301	1
Fagron	Chloral hydrate	17J31-B02-342155	2
Fagron	Chloral hydrate	18F15-B01-355393	2
Fagron	Chloral hydrate	18F15-B01-355394	2
Fagron	Chloral hydrate	18L18-B01-193679	1
Fagron	Chloral hydrate	192872002	1
Fagron	Chloral hydrate	19K04-B01	1
Fagron	Chloral hydrate	19K04-B01-1955569	1
Fagron	Chloral hydrate	19K04-B01-195569	1
Fagron	Chloral hydrate	19K04-B01-201434	3
Fagron	Chloral hydrate	21001025016	1
Fagron	Chloral hydrate	21B25-B03-203396	2
Gehe amax	Chloral hydrate	19000511001	1
Gehe	Chloral hydrate	15083703	1
GEHE	Chloral hydrate	15448312	1
Gehe	Chloral hydrate	15448326	1
Gehe	Chloral hydrate	17247704	2
Gehe	Chloral hydrate	17346301	1
Gehe	Chloral hydrate	192872001	1
Gehe	Chloral hydrate	2000232302	1
Gehe	Chloral hydrate	22004038001	1
Gehe	Chloral hydrate	24002447005	1
Ichthyol GmBH	Chloral hydrate	13002425	2
Ichthyol	Chloral hydrate	15448314	1
Jenne	Chloral hydrate	21001025020	1
Kehr	Chloral hydrate	17346302	1
Kehr	Chloral hydrate	22004038001	2
L12	Chloral hydrate	17346301	1
Noweda	Chloral hydrate	17314319	1
Noweda	Chloral hydrate	17346306	1
Noweda	Chloral hydrate	17346310	1
Noweda	Chloral hydrate	19091404	1
Noweda	Chloral hydrate	19091408	1
Noweda	Chloral hydrate	19287201	1
Noweda	Chloral hydrate	22004038001	1
Noweda29.04.2015	Chloral hydrate	15083701	2
Phoenix	Chloral hydrate	15448318	1
Phoenix	Chloral hydrate	3187	1
Phönix Gotha	Chloral hydrate	13F06-N07	2
Phönix Gotha	Chloral hydrate	14038302	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Chloral hydrate	17346301	1
Phönix	Chloral hydrate	17346303	3
Phönix	Chloral hydrate	17346311	5
Phönix	Chloral hydrate	192872001	1
Phönix	Chloral hydrate	22004038001	2
Phönix	Chloral hydrate	2202204038007	1
Sanacorp	Chloral hydrate	12H06-N08	3
Sanacorp	Chloral hydrate	14218705	1
Sanacorp	Chloral hydrate	15448326	1
Sanacorp	Chloral hydrate	17346301	1
Sanacorp	Chloral hydrate	17346306	1
Sanacorp	Chloral hydrate	192872001	1
Sanacorp	Chloral hydrate	21001025002	2
Sanacorp	Chloral hydrate	21001025007	1
Sanacorp	Chloral hydrate	21001025023	3
Sanacorp	Chloral hydrate	22004038001	2
Sanacorp	Chloral hydrate	22004038007	1

- 234 976 spectra from 1515 *Apo-Ident* customers from a total of 49 064 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Chloral hydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Chloral hydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	240	0	152 722
Type B	0	530	0	201 554
Type C	0	1063	28	234 976

The substance/substance group *Chloral hydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8679 %)
Type C	100.0000 % (> 99.9007 %)	97.4335 % (> 97.1586 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21231	22963	13.12	153.80
21309	22963	6.67	154.57
22963	22963	0.00	148.74
23094	22963	7.61	153.47
23572	22963	5.55	151.56
25488	22963	11.12	156.00

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Chloramphenicol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20097-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Chloramphenicol; Chloramphenicolum

Special notes

When selecting the *Chloramphenicol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Chloramphenicol	10	14	333

Second-stage model

For differentiation of the substance/substance group *Chloramphenicol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Chloramphenicol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Oxytetracycline hydrochloride	87.17	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Chloramphenicol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Chloramphenicol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Chloramphenicol	11370716	20787	40	20120202
Caelo	Chloramphenicol	12248507	20807	40	20120831
Caelo	Chloramphenicol	13080924	21701	60	1509287
Caelo	Chloramphenicol	14346908	21988	60	20150115
Euro OTC	Chloramphenicol	1209019-02	20813	80	20130408
Euro OTC	Chloramphenicol	1209019-02	20815	80	20130408
Euro OTC	Chloramphenicol	1407043-01	21752	60	20140903
Euro OTC	Chloramphenicol	1602002	22367	45	20160309*
Fagron	Chloramphenicol	11F20-N05	20777	120	1412249
Fagron	Chloramphenicol	13A11-N02	20822	40	20130125
Fagron	Chloramphenicol	14E01-B02-308559	21910	60	20140513

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 685 spectra of 11 reference samples from the substance/substance group *Chloramphenicol*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 277 spectra from a total of 2832 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 610 spectra of 17 reference samples from the substance/substance group *Chloramphenicol*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Chloramphenicol	15358906	22961	40
Caelo	Chloramphenicol	162786	23353	40
Caelo	Chloramphenicol	180178	24049	40
Caelo	Chloramphenicol	192260	24892	40
Caelo	Chloramphenicol	20000261	25211	40
Caelo	Chloramphenicol	22002986	26495	40
Caelo	Chloramphenicol	24001644	27439	40
Euro OTC	Chloramphenicol	1704021	23392	40
Euro OTC	Chloramphenicol	1903028	24625	40
Euro OTC	Chloramphenicol	2002043	25264	40
Euro OTC	Chloramphenicol	2201014	25958	40
Euro OTC	Chloramphenicol	2306004	26924	40
Euro OTC	Chloramphenicol	2403008	27362	40
Fagron	Chloramphenicol	22B02-B09-219706	26158	40
Caelo	Chloramphenicol	22002986	26495SI	20
Euro OTC	Chloramphenicol	2201014	25958SI	10
Fagron	Chloramphenicol	22B02-B09-219706	26158SI	20

- 201 474 spectra from a total of 4031 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3293 spectra from 977 *Apo-Ident* customers from 347 batches from the substance/substance group *Chloramphenicol*.

- Among them are spectra of independent samples from 330 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Chloramphenicol	2002043-03	1
	Chloramphenicol	21001144006	1
	Chloramphenicol	21001144009	1
	Chloramphenicol	21001144014	1
	Chloramphenicol	220002986002	1
	Chloramphenicol	22002986001	8
	Chloramphenicol	22002986002	2
	Chloramphenicol	22002986003	8
	Chloramphenicol	22002986006	2
	Chloramphenicol	22002986007	8
	Chloramphenicol	2201014-01	7
	Chloramphenicol	2201014-02	13
	Chloramphenicol	2201014-03	7
	Chloramphenicol	220101404	1
	Chloramphenicol	2201014-04	3
	Chloramphenicol	220104-02	1
	Chloramphenicol	221014-01	1
	Chloramphenicol	2306004-01	11
	Chloramphenicol	2306004-02	1
	Chloramphenicol	2403008-01	1
	Chloramphenicol	DY0092000082	1
4,64	Chloramphenicol	1903028-03	1
AHD	Chloramphenicol	12248507	1
AHD	Chloramphenicol	12248509	1
AHD	Chloramphenicol	13080904	1
AHD	Chloramphenicol	14346912	1
AHD	Chloramphenicol	18017807	1
AHD	Chloramphenicol	2306004-01	1
AHD	Chloramphenicol	2306004-02	2
AHDE 20.08.15	Chloramphenicol	DY00912128	1
Alliance 15.04.2015 ...	Chloramphenicol	1407043-01	1
Alliance Health	Chloramphenicol	1209019-02	1
Alliance Healthcare	Chloramphenicol	21001144009	1
Anzag 03.04.13 ek: 3,18EUR	Chloramphenicol	12248501	1
Anzag ek:2.98EUR 25.08.12	Chloramphenicol	11370711	1
Anzag	Chloramphenicol	1302024-01	1
Anzag	Chloramphenicol	1308017-02	1
ANZAG	Chloramphenicol	1308017-02	1
Anzag	Chloramphenicol	14346924	2
anzag	Chloramphenicol	15358907	1
Anzag	Chloramphenicol	1602002-03	1
apo-ident	Chloramphenicol	1602002-03	1
Audor Pharma	Chloramphenicol	2002043/01	1
Audor Pharma	Chloramphenicol	2201014-01	1
Beiersdorf	Chloramphenicol	1704021-03	1
Bombastus	Chloramphenicol	1308017-01	1
Bombastus	Chloramphenicol	1602002-03	1
Bombastus	Chloramphenicol	1704021-01	1
Bombastus	Chloramphenicol	2002043-01	3
Caelo	Chloramphenicol		1
Caelo	Chloramphenicol	10341703	1
Caelo	Chloramphenicol	10341707	1
Caelo	Chloramphenicol	10341711	2
Caelo	Chloramphenicol	10341717	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Chloramphenicol	1062002-04	1
Caelo	Chloramphenicol	11031402	1
Caelo	Chloramphenicol	1137004	1
Caelo	Chloramphenicol	1137070	1
Caelo	Chloramphenicol	11370702	3
Caelo	Chloramphenicol	11370703	2
Caelo	Chloramphenicol	11370705	3
Caelo	Chloramphenicol	11370706	3
Caelo	Chloramphenicol	11370707	2
Caelo	Chloramphenicol	11370711	12
Caelo	Chloramphenicol	11370712	4
Caelo	Chloramphenicol	11370713	3
Caelo	Chloramphenicol	11370714	2
Caelo	Chloramphenicol	11370715	1
Caelo	Chloramphenicol	11370716	4
Caelo	Chloramphenicol	11370717	2
Caelo	Chloramphenicol	1137714	1
Caelo	Chloramphenicol	1203012-02	1
Caelo	Chloramphenicol	12072606	1
Caelo	Chloramphenicol	12248501	12
Caelo	Chloramphenicol	12248505	2
Caelo	Chloramphenicol	12248506	8
Caelo	Chloramphenicol	12248507	9
Caelo	Chloramphenicol	12248509	12
Caelo	Chloramphenicol	12248520	7
Caelo	Chloramphenicol	12248524	7
Caelo	Chloramphenicol	12248525	7
Caelo	Chloramphenicol	12g02n01	1
Caelo	Chloramphenicol	12G02-N01	2
Caelo	Chloramphenicol	1302024-01	1
Caelo	Chloramphenicol	1302024-02	2
Caelo	Chloramphenicol	130416-1	1
Caelo	Chloramphenicol	130416-2	1
Caelo	Chloramphenicol	1308017-01	1
Caelo	Chloramphenicol	13080303	1
Caelo	Chloramphenicol	130809	1
Caelo	Chloramphenicol	13080902	1
Caelo	Chloramphenicol	13080903	8
Caelo	Chloramphenicol	13080904	5
Caelo	Chloramphenicol	13080907	13
Caelo	Chloramphenicol	13080908	4
Caelo	Chloramphenicol	13080915	1
Caelo	Chloramphenicol	13080917	4
Caelo	Chloramphenicol	13080918	2
Caelo	Chloramphenicol	13080921	4
Caelo	Chloramphenicol	13080923	13
Caelo	Chloramphenicol	13080924	15
Caelo	Chloramphenicol	13080925	11
Caelo	Chloramphenicol	13A31-B02	1
Caelo	Chloramphenicol	13A31-B02-286709	1
Caelo	Chloramphenicol	140704301	2
Caelo	Chloramphenicol	1407043-01	1
Caelo	Chloramphenicol	14246917	1
Caelo	Chloramphenicol	1434608	1
Caelo	Chloramphenicol	14346901	2
Caelo	Chloramphenicol	14346903	1
Caelo	Chloramphenicol	14346904	4
Caelo	Chloramphenicol	14346906	4
Caelo	Chloramphenicol	14346907	9
Caelo	Chloramphenicol	14346908	10

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Chloramphenicol	14346910	15
Caelo	Chloramphenicol	14346911	22
Caelo	Chloramphenicol	14346912	3
Caelo	Chloramphenicol	14346913	8
Caelo	Chloramphenicol	14346914	4
Caelo	Chloramphenicol	14346917	8
Caelo	Chloramphenicol	14346918	18
Caelo	Chloramphenicol	14346918I-080816-1	1
Caelo	Chloramphenicol	14346922	1
Caelo	Chloramphenicol	14346924	5
Caelo	Chloramphenicol	14356910	1
Caelo	Chloramphenicol	1436908	1
Caelo	Chloramphenicol	1436918	1
Caelo	Chloramphenicol	14E01-B02-296623	1
Caelo	Chloramphenicol	14E01B02296624	1
Caelo	Chloramphenicol	14E01-B02-308559	2
Caelo	Chloramphenicol	14EO01-B02	1
Caelo	Chloramphenicol	1502036-01	3
Caelo	Chloramphenicol	1502036-02	2
Caelo	Chloramphenicol	150203603	1
Caelo	Chloramphenicol	1502036-03	2
Caelo	Chloramphenicol	150528C	1
Caelo	Chloramphenicol	153589	1
Caelo	Chloramphenicol	15358903	3
Caelo	Chloramphenicol	15358905	25
Caelo	Chloramphenicol	15358906	13
Caelo	Chloramphenicol	15358907	3
Caelo	Chloramphenicol	15358908	10
Caelo	Chloramphenicol	15358909	6
Caelo	Chloramphenicol	15358911	1
Caelo	Chloramphenicol	15358912	14
Caelo	Chloramphenicol	15358913	28
Caelo	Chloramphenicol	15358914	21
Caelo	Chloramphenicol	1535896	1
Caelo	Chloramphenicol	160200201	1
Caelo	Chloramphenicol	1602002-01	5
Caelo	Chloramphenicol	1602002-02	2
Caelo	Chloramphenicol	1602002-03	1
Caelo	Chloramphenicol	16258612	1
Caelo	Chloramphenicol	16278009	1
Caelo	Chloramphenicol	16278601	1
Caelo	Chloramphenicol	16278602	9
Caelo	Chloramphenicol	16278605	1
Caelo	Chloramphenicol	16278606	12
Caelo	Chloramphenicol	16278608	18
Caelo	Chloramphenicol	16278609	29
Caelo	Chloramphenicol	16278609/180420CA	1
Caelo	Chloramphenicol	16278610	1
Caelo	Chloramphenicol	16278611	2
Caelo	Chloramphenicol	16278612	31
Caelo	Chloramphenicol	1627862	1
Caelo	Chloramphenicol	1627898	1
Caelo	Chloramphenicol	16358909	1
Caelo	Chloramphenicol	170402101	1
Caelo	Chloramphenicol	1704021-01	18
Caelo	Chloramphenicol	1704021-02	7
Caelo	Chloramphenicol	1704021-03	3
Caelo	Chloramphenicol	1704021-04	8
Caelo	Chloramphenicol	17343802	13
Caelo	Chloramphenicol	17343803	32

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Chloramphenicol	174021-02	2
Caelo	Chloramphenicol	180178	1
Caelo	Chloramphenicol	18017802	6
Caelo	Chloramphenicol	18017804	5
Caelo	Chloramphenicol	18017806	40
Caelo	Chloramphenicol	18017807	14
Caelo	Chloramphenicol	18017809	37
Caelo	Chloramphenicol	18017810	9
Caelo	Chloramphenicol	18017811	20
Caelo	Chloramphenicol	18017813	4
Caelo	Chloramphenicol	18017814	9
Caelo	Chloramphenicol	18025702	2
Caelo	Chloramphenicol	181017809	1
Caelo	Chloramphenicol	1903028-01	10
Caelo	Chloramphenicol	1903028-02	6
Caelo	Chloramphenicol	1903028-041	1
Caelo	Chloramphenicol	19222226003	1
Caelo	Chloramphenicol	19225003	1
Caelo	Chloramphenicol	192260001	3
Caelo	Chloramphenicol	19226001	1
Caelo	Chloramphenicol	19226002	25
Caelo	Chloramphenicol	19226003	99
Caelo	Chloramphenicol	19226003P-200323-1	1
Caelo	Chloramphenicol	19226004	1
Caelo	Chloramphenicol	1922603	1
Caelo	Chloramphenicol	20000261003	8
Caelo	Chloramphenicol	20000261004	37
Caelo	Chloramphenicol	20003760002	12
Caelo	Chloramphenicol	20003760003	55
Caelo	Chloramphenicol	20003760006	5
Caelo	Chloramphenicol	2000376003	1
Caelo	Chloramphenicol	2000376006	1
Caelo	Chloramphenicol	2002043-01	4
Caelo	Chloramphenicol	2002043-02	4
Caelo	Chloramphenicol	200204303	1
Caelo	Chloramphenicol	2003760003	2
Caelo	Chloramphenicol	20102012J1	1
Caelo	Chloramphenicol	21001144003	3
Caelo	Chloramphenicol	21001144004	21
Caelo	Chloramphenicol	21001144006	6
Caelo	Chloramphenicol	21001144007	17
Caelo	Chloramphenicol	21001144010	1
Caelo	Chloramphenicol	21001144014	2
Caelo	Chloramphenicol	2100144004	2
Caelo	Chloramphenicol	21002415002	1
Caelo	Chloramphenicol	2181116	1
Caelo	Chloramphenicol	22002986001	3
Caelo	Chloramphenicol	22002986003	3
Caelo	Chloramphenicol	2201014-01	5
Caelo	Chloramphenicol	28011401	1
Caelo	Chloramphenicol	3081602	1
Caelo	Chloramphenicol	310311	1
Caelo	Chloramphenicol	3125204	1
Caelo	Chloramphenicol	3217A-01259	1
Caelo	Chloramphenicol	4412Q-01259	1
Caelo	Chloramphenicol	4654572	1
Caelo	Chloramphenicol	4712Q-01259	1
Caelo	Chloramphenicol	8017811	1
Caelo	Chloramphenicol	82853399	1
Caelo	Chloramphenicol	8701	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Chloramphenicol	93323801	1
Caelo	Chloramphenicol	DY00911233	1
Caelo	Chloramphenicol	DY00916161	1
Caelo	Chloramphenicol	DY130525	2
Caeol/Noweda	Chloramphenicol	19226003	2
Caeolo / Anzag	Chloramphenicol	15358914	1
Caeolo	Chloramphenicol	20003760003	4
Caesar & Loretz Gmb	Chloramphenicol	18017814	2
Caesar & Loretz GmbH...	Chloramphenicol	19226003	2
Caesar & Loretz GmbH...	Chloramphenicol	18017809	1
Caesar & Loretz GmbH...	Chloramphenicol	18017811	1
Caesar & Loretz GmbH...	Chloramphenicol	20000261004	1
Caesar & Loretz GmbH...	Chloramphenicol	21001144004	2
Caesar & Loretz GmbH...	Chloramphenicol	20003760002	1
Caesar & Loretz GmbH...	Chloramphenicol	21001144004	1
Caesar & Loretz GmbH...	Chloramphenicol	22002986001	1
Caesar & Loretz GmbH...	Chloramphenicol	19226003	1
Caesar & Loretz GmbH...	Chloramphenicol	20000261003	1
Caesar & Loretz GmbH...	Chloramphenicol	20003760002	1
Caesar & Loretz GmbH...	Chloramphenicol	19226003	1
Caesar & Loretz GmbH...	Chloramphenicol	21001144007	2
Caesar & Loretz GmbH...	Chloramphenicol	21001144004	1
Caesar & Loretz GmbH...	Chloramphenicol	18017809	1
Caesar & Loretz GmbH...	Chloramphenicol	20003760003	3
Caesar & Loretz GmbH/Gehe	Chloramphenicol	18017811	2
Caesar & Loretz GmbH/Gehe	Chloramphenicol	20003760002	1
Caesar & Loretz GmbH/Gehe	Chloramphenicol	21001144007	1
Caesar & Loretz GmbH...	Chloramphenicol	20003760003	1
Caesar & Loretz GmbH...	Chloramphenicol	19226002	1
Caesar & Loretz GmbH...	Chloramphenicol	20000261004	1
Caesar & Loretz GmbH...	Chloramphenicol	20003760003	1
Caesar & Loretz GmbH...	Chloramphenicol	192260001	1
Caesar & Loretz GmbH/Otto	Chloramphenicol	19226003	1
Caesar & Loretz GmbH...	Chloramphenicol	18017814	1
Caesar & Loretz GmbH...	Chloramphenicol	20000261004	1
Caesar & Loretz GmbH...	Chloramphenicol	20003760003	3
Caesar & Loretz GmbH...	Chloramphenicol	20000261004	2
Caesar & Loretz GmbH...	Chloramphenicol	20003760003	1
Caesar & Loretz GmbH...	Chloramphenicol	21001144004	1
Caesar & Loretz GmbH...	Chloramphenicol	18017811	1
Caesar & Loretz GmbH	Chloramphenicol	11370711	1
Caesar & Loretz GmbH	Chloramphenicol	18017806	1
Caesar & Loretz GmbH	Chloramphenicol	18017809	6
Caesar & Loretz GmbH	Chloramphenicol	18017810	2
Caesar & Loretz GmbH	Chloramphenicol	18017811	10
Caesar & Loretz GmbH	Chloramphenicol	18017813	1
Caesar & Loretz GmbH	Chloramphenicol	18017814	3
Caesar & Loretz GmbH	Chloramphenicol	1903028-01	1
Caesar & Loretz GmbH	Chloramphenicol	1903028-02	3
Caesar & Loretz GmbH	Chloramphenicol	192260001	1
Caesar & Loretz GmbH	Chloramphenicol	19226001	1
Caesar & Loretz GmbH	Chloramphenicol	19226002	12
Caesar & Loretz GmbH	Chloramphenicol	19226003	57
Caesar & Loretz GmbH	Chloramphenicol	19226004	2
Caesar & Loretz GmbH	Chloramphenicol	20000261003	3
Caesar & Loretz GmbH	Chloramphenicol	20000261004	9
Caesar & Loretz GmbH	Chloramphenicol	20003343004	1
Caesar & Loretz GmbH	Chloramphenicol	20003760002	5
Caesar & Loretz GmbH	Chloramphenicol	20003760003	28
Caesar & Loretz GmbH	Chloramphenicol	20003760006	8

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Chloramphenicol	2000376003	1
Caesar & Loretz GmbH	Chloramphenicol	21001144004	18
Caesar & Loretz GmbH	Chloramphenicol	21001144006	2
Caesar & Loretz GmbH	Chloramphenicol	21001144007	11
Caesar & Loretz GmbH	Chloramphenicol	21001144009	1
Caesar & Loretz GmbH	Chloramphenicol	21001144014	2
Caesar & Loretz GmbH	Chloramphenicol	22002986001	2
Caesar & Loretz	Chloramphenicol	15358908	1
Caesar & Loretz	Chloramphenicol	16278609	2
Caesar & Loretz	Chloramphenicol	18017809	1
Caesar & Loretz	Chloramphenicol	21001144004	1
Caesar & Loretz	Chloramphenicol	21001144014	1
Caesar&Lorenz	Chloramphenicol	20003760003	1
Caesar&Loretz	Chloramphenicol	16278612	1
Caeser und Loretz GmbH	Chloramphenicol	19226002	1
Caleo/ Noweda	Chloramphenicol	173436803	1
Caolo- Noweda	Chloramphenicol	14346908	1
Cealo/Gehe	Chloramphenicol	2100114406	3
Cealo	Chloramphenicol	1602002-03	1
Chloramphenicol	Chloramphenicol	2002043-01	1
Eu Rho Pharm/E	Chloramphenicol	1903028-02	1
Eu Rho Pharm/K	Chloramphenicol	1704021-04	1
Eur Rho Phönix	Chloramphenicol	2002043-02	1
EuRho / 20	Chloramphenicol	1502036-01	1
EuRho / Noweda	Chloramphenicol	1903028-02	1
Eurho No	Chloramphenicol	1903028-01	1
EuRho Noweda	Chloramphenicol	2002043-01	1
Eurho ph	Chloramphenicol	1903028-02	1
Eurho Phönix	Chloramphenicol	1704021-02	1
Eurho Phönix	Chloramphenicol	2002043-02	2
EuRho/ Phönix	Chloramphenicol	1704021-01	2
EuRho/ Phönix	Chloramphenicol	20002043-01	1
EuRho/ Sanacorp	Chloramphenicol	2002043-02	1
Eurho/AHD	Chloramphenicol	2002043-02	1
EuRho/Alliance	Chloramphenicol	2002043-01	1
EuRho/Gehe	Chloramphenicol	1704021-04	1
EuRho/Gehe	Chloramphenicol	1903028-02	1
EuRho/Gehe	Chloramphenicol	2002043-01	1
EuRho/Gehe	Chloramphenicol	919110016	1
EuRho/Noweda	Chloramphenicol	1704021-02	1
EuRho/Noweda	Chloramphenicol	2002043-02	1
EuRho/Phoenix	Chloramphenicol	2002043-01	3
EuRho/Phoenix	Chloramphenicol	2201014-03	1
EuRho/Phönix	Chloramphenicol	123012-01	1
EuRho/Phönix	Chloramphenicol	1308017-01	1
EuRho/Phönix	Chloramphenicol	1903028-02	1
Eurho/Phönix	Chloramphenicol	2002043-01	1
EuRho/Phönix	Chloramphenicol	2002043-01	1
EuRho/Sanacorp	Chloramphenicol	1704021-01	1
EuRho/Sanacorp	Chloramphenicol	2002043-03	2
EuRho	Chloramphenicol	1308017-02	1
EuRho	Chloramphenicol	15358913	1
EuRho	Chloramphenicol	1704021-01	2
EuRho	Chloramphenicol	1704021-02	2
EuRho	Chloramphenicol	1704021-03	2
EuRho	Chloramphenicol	1704021-04	1
Eurho	Chloramphenicol	1704087-03	1
EuRho	Chloramphenicol	1903028-01	2
Eurho	Chloramphenicol	1903028-02	1
EuRho	Chloramphenicol	1903028-02	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho	Chloramphenicol	2002043-01	4
EuRho	Chloramphenicol	2002043-02	3
euRho	Chloramphenicol	2002043-03	2
Eurho	Chloramphenicol	2002043-03	1
EuRho	Chloramphenicol	2002043-03	2
EuRho	Chloramphenicol	2002043-1	1
EuRho	Chloramphenicol	216A-01259	1
Euro OCT / Krieger	Chloramphenicol	2002043-01	1
Euro OCT	Chloramphenicol	1203012-02	1
Euro OTC	Chloramphenicol		5
Euro OTC	Chloramphenicol	10061707	1
Euro OTC	Chloramphenicol	1012013-01	2
Euro OTC	Chloramphenicol	1107002-01	2
Euro OTC	Chloramphenicol	110700202	1
Euro OTC	Chloramphenicol	1107002-02	1
Euro OTC	Chloramphenicol	120250	1
Euro OTC	Chloramphenicol	1203012-01	7
Euro OTC	Chloramphenicol	1203012-02	12
Euro OTC	Chloramphenicol	1203012-12	1
Euro OTC	Chloramphenicol	1209010-02	3
Euro OTC	Chloramphenicol	1209019-01	6
Euro OTC	Chloramphenicol	120901902	3
Euro OTC	Chloramphenicol	1209019-02	11
Euro OTC	Chloramphenicol	1302024-01	12
Euro OTC	Chloramphenicol	1302024-02	7
Euro OTC	Chloramphenicol	130801701	1
Euro OTC	Chloramphenicol	1308017-01	10
Euro OTC	Chloramphenicol	130801702	2
Euro OTC	Chloramphenicol	1308017-02	11
Euro OTC	Chloramphenicol	13111410	1
Euro OTC	Chloramphenicol	1317M-01259	1
Euro OTC	Chloramphenicol	1407043	1
Euro OTC	Chloramphenicol	140704301	5
Euro OTC	Chloramphenicol	1407043-01	24
Euro OTC	Chloramphenicol	14101717	1
Euro OTC	Chloramphenicol	14346910	1
Euro OTC	Chloramphenicol	1502036	1
Euro OTC	Chloramphenicol	150203601	5
Euro OTC	Chloramphenicol	1502036-01	34
Euro OTC	Chloramphenicol	150203602	2
Euro OTC	Chloramphenicol	1502036-02	19
Euro OTC	Chloramphenicol	1502036022016030911	1
Euro OTC	Chloramphenicol	150203603	1
Euro OTC	Chloramphenicol	1502036-03	25
Euro OTC	Chloramphenicol	1502063-02	1
Euro OTC	Chloramphenicol	1509211259	1
Euro OTC	Chloramphenicol	15358906	1
Euro OTC	Chloramphenicol	15358914	4
Euro OTC	Chloramphenicol	16020002-02	1
Euro OTC	Chloramphenicol	16020002-03	1
Euro OTC	Chloramphenicol	1602002-01	43
Euro OTC	Chloramphenicol	1602002-02	28
Euro OTC	Chloramphenicol	160200203	2
Euro OTC	Chloramphenicol	1602002-03	41
Euro OTC	Chloramphenicol	1602002-04	2
Euro OTC	Chloramphenicol	1602002-07	1
Euro OTC	Chloramphenicol	1701021-04	1
Euro OTC	Chloramphenicol	1704021	4
Euro OTC	Chloramphenicol	1704021_02	1
Euro OTC	Chloramphenicol	170402101	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Chloramphenicol	1704021-01	102
Euro OTC	Chloramphenicol	1704021-015505	1
Euro OTC	Chloramphenicol	1704021-01A	1
Euro OTC	Chloramphenicol	170402102	1
Euro OTC	Chloramphenicol	1704021-02	58
Euro OTC	Chloramphenicol	170402103	3
Euro OTC	Chloramphenicol	1704021-03	50
Euro OTC	Chloramphenicol	170402104	2
Euro OTC	Chloramphenicol	1704021-04	73
Euro OTC	Chloramphenicol	17040212-04	1
Euro OTC	Chloramphenicol	170421-01	1
Euro OTC	Chloramphenicol	17044021-01	1
Euro OTC	Chloramphenicol	1707021-02	1
Euro OTC	Chloramphenicol	17704021-01	1
Euro OTC	Chloramphenicol	18017802	1
Euro OTC	Chloramphenicol	18017809	2
Euro OTC	Chloramphenicol	180178091903028-01	1
Euro OTC	Chloramphenicol	1903028	7
Euro OTC	Chloramphenicol	1903028_01	1
Euro OTC	Chloramphenicol	190302801	6
Euro OTC	Chloramphenicol	1903028-01	128
Euro OTC	Chloramphenicol	1903028-010	1
Euro OTC	Chloramphenicol	190302802	1
Euro OTC	Chloramphenicol	1903028-02	105
Euro OTC	Chloramphenicol	190302803	1
Euro OTC	Chloramphenicol	1903028-03	30
Euro OTC	Chloramphenicol	1903028-42	1
Euro OTC	Chloramphenicol	191210111	1
Euro OTC	Chloramphenicol	193028-03	1
Euro OTC	Chloramphenicol	20012043-02	1
Euro OTC	Chloramphenicol	2002043	3
Euro OTC	Chloramphenicol	200204301	2
Euro OTC	Chloramphenicol	2002043-01	102
Euro OTC	Chloramphenicol	2002043-01/4420	1
Euro OTC	Chloramphenicol	200204302	5
Euro OTC	Chloramphenicol	2002043-02	142
Euro OTC	Chloramphenicol	200204303	4
Euro OTC	Chloramphenicol	2002043-03	45
Euro OTC	Chloramphenicol	2002043-1	1
Euro OTC	Chloramphenicol	20022043-01	1
Euro OTC	Chloramphenicol	200243-02	2
Euro OTC	Chloramphenicol	2004030-01	1
Euro OTC	Chloramphenicol	211217(2002043-01)	1
Euro OTC	Chloramphenicol	2121211203012-0	1
Euro OTC	Chloramphenicol	2201014-01	31
Euro OTC	Chloramphenicol	2201014-02	10
Euro OTC	Chloramphenicol	2201014-04	2
Euro OTC	Chloramphenicol	22010144-01	1
Euro OTC	Chloramphenicol	221014-02	1
Euro OTC	Chloramphenicol	2306004-01	1
Euro OTC	Chloramphenicol	314Q1259	1
Euro OTC	Chloramphenicol	90302801	1
Euro OTC	Chloramphenicol	916161	1
Euro OTC	Chloramphenicol	919110016	6
Euro OTC	Chloramphenicol	DY00912128	6
Euro OTC	Chloramphenicol	DY00914151	1
Euro OTC	Chloramphenicol	DY00918024	1
Euro OTC	Chloramphenicol	DY00918024/1903028-02	1
Euro OTC	Chloramphenicol	DY0092000082	2
Euro OTC	Chloramphenicol	DY130525	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Chloramphenicol	T02-55/1407043-01	1
Euro OTG	Chloramphenicol	1502036-01	1
euro pharm	Chloramphenicol	1602002-01	1
Euro/ Sanacorp	Chloramphenicol	1308017-02	1
Euro//Sanacorp	Chloramphenicol	2002043-01	1
EUro/AHD	Chloramphenicol	1209019-01	1
EUro/AHD	Chloramphenicol	1209019-02	1
Euro/Alliance Healthcare	Chloramphenicol	1502036-01	1
Euro/Krieger	Chloramphenicol	1602002-02	1
Euro/Krieger	Chloramphenicol	1602002-03	1
Euro/Noweda	Chloramphenicol	1602002-02	1
Euro/Phönix	Chloramphenicol	1502036-03	1
Euro/Phönix	Chloramphenicol	1704021-02	1
Euro/Phönix	Chloramphenicol	1704021-04	1
Euro/Phönix	Chloramphenicol	1903028-01	1
euro	Chloramphenicol	2002043-01	1
EurPS	Chloramphenicol	1502036-01	2
Fagron	Chloramphenicol		2
Fagron	Chloramphenicol	11/14-N03	2
Fagron	Chloramphenicol	11J14-N03	1
Fagron	Chloramphenicol	120250-0002	1
Fagron	Chloramphenicol	1202500003	1
Fagron	Chloramphenicol	12A11-N02	1
Fagron	Chloramphenicol	12B13-N06	6
Fagron	Chloramphenicol	12F01-N23	1
Fagron	Chloramphenicol	12G02-N01	9
Fagron	Chloramphenicol	12L11-N06	9
Fagron	Chloramphenicol	13A11N02	1
Fagron	Chloramphenicol	13A11-N02	6
Fagron	Chloramphenicol	13A31-B02	8
Fagron	Chloramphenicol	13A31-B02_286708	1
Fagron	Chloramphenicol	13A31-B02-286708	4
Fagron	Chloramphenicol	13A31-B02-286709	2
Fagron	Chloramphenicol	13A31-B02-290263	1
Fagron	Chloramphenicol	13A31-B02-290300	4
Fagron	Chloramphenicol	14E01-B02	5
Fagron	Chloramphenicol	14E01-B02_296624	1
Fagron	Chloramphenicol	14E01-B02-296623	1
Fagron	Chloramphenicol	14e01-b02-296624	1
Fagron	Chloramphenicol	14E01B02296624	2
Fagron	Chloramphenicol	14E01-B02-296624	7
Fagron	Chloramphenicol	14E01-B02-296625	1
Fagron	Chloramphenicol	14E01-B02-306146	7
Fagron	Chloramphenicol	14E01-B02-308559	7
Fagron	Chloramphenicol	1502036-01	1
Fagron	Chloramphenicol	15358914	1
Fagron	Chloramphenicol	1602002-01	2
Fagron	Chloramphenicol	1602002-02	1
Fagron	Chloramphenicol	1602002-03	1
Fagron	Chloramphenicol	1612-B07-329313	1
Fagron	Chloramphenicol	1704021-01	1
Fagron	Chloramphenicol	1903028-01	1
Fagron	Chloramphenicol	1903028-02	1
Fagron	Chloramphenicol	2002043-01	2
Fagron	Chloramphenicol	20E14-B19-202352	2
Fagron	Chloramphenicol	2111I-01259	1
Fagron	Chloramphenicol	DY00911233	4
Fagron	Chloramphenicol	DY00912129	1
Fagron	Chloramphenicol	LTOCHL/049/16-17M	1
Fiebig	Chloramphenicol	1502036-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fiebig	Chloramphenicol	15358913	1
Fiebig	Chloramphenicol	1602002-01	1
Fiebig	Chloramphenicol	16278608	1
Fiebig	Chloramphenicol	16278609	1
Fiebig	Chloramphenicol	16278612	1
Fiebig	Chloramphenicol	1704021-01	1
Fiebig	Chloramphenicol	1734803	1
Fiebig	Chloramphenicol	18017809	1
Fiebig	Chloramphenicol	18017810	1
Fiebig	Chloramphenicol	19226002	1
Finteler Apotheke	Chloramphenicol	15358913	1
Fischar/Sanacorp	Chloramphenicol	1704021-04	1
Fischer/ Noweda	Chloramphenicol	1502036-03	1
Fragon	Chloramphenicol	12G02-N01	1
Gatt-Koller / Phoenix	Chloramphenicol	5615/12115211	1
Gehe - Hedinger	Chloramphenicol	1704021-01	1
Gehe 27.06.15/euro	Chloramphenicol	1502036-01	2
Gehe amax	Chloramphenicol	1602002-03	1
gehe/ Northeast Pharma	Chloramphenicol	2002043-01	1
Gehe	Chloramphenicol	1107002-02	1
Gehe	Chloramphenicol	1203012-01	1
Gehe	Chloramphenicol	1209019-02	1
Gehe	Chloramphenicol	1308017-02	1
Gehe	Chloramphenicol	14346910	1
Gehe	Chloramphenicol	15358906	1
Gehe	Chloramphenicol	15358909	1
Gehe	Chloramphenicol	15358913	2
GEHE	Chloramphenicol	15358914	1
GEHE	Chloramphenicol	160200202	1
GEHE	Chloramphenicol	16278608	1
Gehe	Chloramphenicol	16278612	1
Gehe	Chloramphenicol	17021-04	1
Gehe	Chloramphenicol	1704021-01	3
Gehe	Chloramphenicol	1704021-02	3
Gehe	Chloramphenicol	1704021-03	2
Gehe	Chloramphenicol	1704021-04	1
GEHE	Chloramphenicol	17343803	1
GEHE	Chloramphenicol	18017806	1
Gehe	Chloramphenicol	18017811	1
GEHE	Chloramphenicol	18017811	1
Gehe	Chloramphenicol	1903028_02	1
Gehe	Chloramphenicol	1903028-01	6
Gehe	Chloramphenicol	1903028-02	1
Gehe	Chloramphenicol	1903028-03	1
GEHE	Chloramphenicol	19226002	1
Gehe	Chloramphenicol	19226003	1
Gehe	Chloramphenicol	2002043-01	1
Gehe	Chloramphenicol	2002043-02	1
Gehe	Chloramphenicol	22002986007	1
Gehe	Chloramphenicol	2201014-01	1
GEHE	Chloramphenicol	2201014-02	1
GEHE	Chloramphenicol	2201014-03	1
Gutenberg-Apotheke	Chloramphenicol	13A31-B02-286710	1
Jenne	Chloramphenicol	1903028	1
Jenne	Chloramphenicol	200204301	1
Jenne	Chloramphenicol	2002043-02	1
Kehr	Chloramphenicol	1704021-01	1
Kehr	Chloramphenicol	22002986001	1
Kehr	Chloramphenicol	22005298	1
Kehr	Chloramphenicol	2200986001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Mehta API	Chloramphenicol	181113082	1
Nanjing / Gehe	Chloramphenicol	14346910	1
Nanjing Baijingyu Ph...	Chloramphenicol	14346917	1
Nanjing Baijingyu Ph...	Chloramphenicol	13080908	2
NanjingBajingyu	Chloramphenicol	1538914	1
Northeast Gen	Chloramphenicol	DY122127	1
Northeast General / Gehe	Chloramphenicol	1602002-02	1
Northeast General/Noweda	Chloramphenicol	1502036-02	1
Northeast General	Chloramphenicol	1407043-01	1
Northeast General	Chloramphenicol	1602002-02	1
Northeast General	Chloramphenicol	1704021-01	2
Northeast General	Chloramphenicol	DY00914151	2
Northeast/Noweda	Chloramphenicol	DY00918024	1
Noweda/EuRho	Chloramphenicol	2002043-01	1
Noweda	Chloramphenicol	1137014	1
Noweda	Chloramphenicol	11370712	1
Noweda	Chloramphenicol	12248509	1
noweda	Chloramphenicol	13080908	2
Noweda	Chloramphenicol	14346901	2
Noweda	Chloramphenicol	14346910	1
Noweda	Chloramphenicol	1502036-03	1
Noweda	Chloramphenicol	15358906	1
Noweda	Chloramphenicol	15358914	1
Noweda	Chloramphenicol	1602002-02	1
Noweda	Chloramphenicol	16278609	1
Noweda	Chloramphenicol	1704021-01	3
Noweda	Chloramphenicol	1704021-02	2
Noweda	Chloramphenicol	1903028	2
Noweda	Chloramphenicol	1903028-01	1
Noweda	Chloramphenicol	1903028-02	1
Noweda	Chloramphenicol	192260001	1
Noweda	Chloramphenicol	19226002	1
Noweda	Chloramphenicol	2002043-02	1
noweda	Chloramphenicol	22002986002	1
Noweda	Chloramphenicol	22002986002	1
Noweda	Chloramphenicol	22002986003	1
NOWEDA	Chloramphenicol	22002986003	1
Noweda	Chloramphenicol	2201014-02	3
Noweda	Chloramphenicol	2201014-04	1
Noweda	Chloramphenicol	220104-01	1
Noweda	Chloramphenicol	2202986003	1
Parthe Apotheke	Chloramphenicol	67/20	1
Ph/Euro	Chloramphenicol	1704021-02	1
Ph/Euro	Chloramphenicol	2002043-03	1
Phoe	Chloramphenicol	15358905	1
PHOENIX 25.04.2014	Chloramphenicol	1308017-02	2
Phoenix	Chloramphenicol	13080903	1
Phoenix	Chloramphenicol	16278609	1
Phoenix	Chloramphenicol	1704021-01	1
phoenix	Chloramphenicol	1704021-02	1
Phoenix	Chloramphenicol	1704021-02	1
Phoenix	Chloramphenicol	18017814	1
phoenix	Chloramphenicol	1903028	1
Phoenix	Chloramphenicol	1903028-01	2
Phoenix	Chloramphenicol	2002043	1
Phoenix	Chloramphenicol	2002043-01	1
Phoenix	Chloramphenicol	200204302	1
Phoenix	Chloramphenicol	2002043-02	1
Phoenix	Chloramphenicol	22002986007	1
Phoenix	Chloramphenicol	2201014-02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Chloramphenicol	2306004-01	1
Phoenix	Chloramphenicol	3087	1
phoenix-06.11.18	Chloramphenicol	17343803	1
Phönix /EURO	Chloramphenicol	2002043-01	1
Phönix 11.11.2019	Chloramphenicol	19226003	1
Phönix 12.10.2019	Chloramphenicol	1903028-01	1
Phönix Gotha	Chloramphenicol	13080907	1
Phönix/Fagon	Chloramphenicol	14346922	1
Phönix	Chloramphenicol	10341710	1
Phönix	Chloramphenicol	10341716	1
Phönix	Chloramphenicol	13080921	1
Phönix	Chloramphenicol	13A11-N02	3
Phönix	Chloramphenicol	13A1-802	3
phönix	Chloramphenicol	15358912	1
PHÖNIX	Chloramphenicol	16278608	1
Phönix	Chloramphenicol	170402103	1
Phönix	Chloramphenicol	18017806	1
Phönix	Chloramphenicol	1903028	1
Phönix	Chloramphenicol	1903028-02	1
Phönix	Chloramphenicol	190328-03	1
Phönix	Chloramphenicol	20003760003	1
Phönix	Chloramphenicol	2002043-01	4
Phönix	Chloramphenicol	2002043-02	2
Phönix	Chloramphenicol	3157	1
Sana 22.11.2017 5.90	Chloramphenicol	16278608	1
Sanacorp 26.09.19 Ek…	Chloramphenicol	1903028-01	2
Sanacorp/EuRho	Chloramphenicol	1704021-02	1
Sanacorp	Chloramphenicol		1
Sanacorp	Chloramphenicol	11370711	1
Sanacorp	Chloramphenicol	120901902	1
Sanacorp	Chloramphenicol	12248501	1
Sanacorp	Chloramphenicol	1308017-02	1
Sanacorp	Chloramphenicol	140704301	1
Sanacorp	Chloramphenicol	1407043-01	2
Sanacorp	Chloramphenicol	1502036-01	1
Sanacorp	Chloramphenicol	15358913	1
Sanacorp	Chloramphenicol	16278612	1
Sanacorp	Chloramphenicol	1704021-01	1
Sanacorp	Chloramphenicol	17343803	1
Sanacorp	Chloramphenicol	18017806	2
Sanacorp	Chloramphenicol	18017809	1
Sanacorp	Chloramphenicol	18017814	2
Sanacorp	Chloramphenicol	1903028-02	2
Sanacorp	Chloramphenicol	19226003	1
Sanacorp	Chloramphenicol	21001144004	1
Sanacorp	Chloramphenicol	22002986001	2
Sanacorp	Chloramphenicol	220101-04	1
Sanacorp	Chloramphenicol	2201014-01	1
sanacorp	Chloramphenicol	2201014-04	1
Sanacorp	Chloramphenicol	2306004-01	1
Sanacorp	Chloramphenicol	41/AKD23	1
Sanacorp	Chloramphenicol	41/AKD24	1
Sannacorp	Chloramphenicol	2201014	1
Spangro 12.05.2014	Chloramphenicol	1308017-01	1
Spangro 14.03.2014	Chloramphenicol	12248524	1
Spangro_22.11.2018	Chloramphenicol	17343803	1
vdl	Chloramphenicol	12248501	1
VDL	Chloramphenicol	1308017-01	1
VDL	Chloramphenicol	140743-01	1

- 232 774 spectra from 1515 *Apo-Ident* customers from a total of 48 919 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Chloramphenicol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Chloramphenicol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	685	0	152 277
Type B	0	610	0	201 474
Type C	0	3288	5	232 774

The substance/substance group *Chloramphenicol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1241 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0164 %)
Type C	100.0000 % (> 99.9007 %)	99.8482 % (> 99.7571 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20777	20777	0.00	178.13
20787	20777	7.27	179.45
20807	20777	4.69	179.09
20813	20777	3.67	178.60
20815	20777	3.66	178.66
20822	20777	3.68	178.41
21701	21701	0.00	184.38
21752	22367	13.27	188.65
21910	22367	3.26	183.89
21988	20777	7.23	181.39
22367	22367	0.00	181.91

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Chlorhexidine diacetate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20989-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Chlorhexidine diacetate; Chlorhexidini acetas

Special notes

When selecting the *Chlorhexidine diacetate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Chlorhexidine diacetate	11	6	137

Second-stage model

For differentiation of the substance/substance group *Chlorhexidine diacetate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Chlorhexidine diacetate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Oxytetracycline hydrochloride	73.04	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Chlorhexidine diacetate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Chlorhexidine diacetate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Chlorhexidine diacetate	12142726	20989	40	1402685
Caelo	Chlorhexidine diacetate	12142727	21041	40	20120711
Caelo	Chlorhexidine diacetate	154389	22456	60	20160309*
Caelo	Chlorhexidine diacetate	15438914	22900	40	1704392
Caelo	Chlorhexidine diacetate	15438914	22951	40	20160309
Caelo	Chlorhexidine diacetate	15438913	23041	40	20160309*
Caelo	Chlorhexidine diacetate	154389	23042	40	20160309*
Caelo	Chlorhexidine diacetate	154389	23043	40	20160309*
Caelo	Chlorhexidine diacetate	15438909	23044	40	20160309*
Caelo	Chlorhexidine diacetate	154389	23048	40	20160309*
Caelo	Chlorhexidine diacetate	22003198	26483	40	20221123*
Caelo	Chlorhexidine diacetate	22003198	26483SI	40	20221123*
Fagron	Chlorhexidine diacetate	14I08-B02-306223	22280	60	20140922
Fagron	Chlorhexidine diacetate	14I08-B02-306223	22280SI	40	20140922
Fagron	Chlorhexidine diacetate	15J02-B08-322916	22946	40	20151104
Fagron	Chlorhexidine diacetate	15J02-B08-322916	22947	40	20151104
Fagron	Chlorhexidine diacetate	22C12-B01-223585	26456	40	20220610
Fagron	Chlorhexidine diacetate	22C12-B01-223585	26456SI	40	20220610
Fagron	Chlorhexidine diacetate	23A26-B06-230994	26816	40	20230313
Fagron	Chlorhexidine diacetate	23A26-B06-230994	26816SI	40	20230313

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 840 spectra of 20 reference samples from the substance/substance group *Chlorhexidine diacetate*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 122 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 475 spectra of 12 reference samples from the substance/substance group *Chlorhexidine diacetate*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Chlorhexidine diacetate	152610	23045	40
Caelo	Chlorhexidine diacetate	171858	23640	40
Caelo	Chlorhexidine diacetate	21001181	25696	50
Caelo	Chlorhexidine diacetate	22000764	26116	35
Caelo	Chlorhexidine diacetate	23001289	26832	30
Fagron	Chlorhexidine diacetate	18A17-B02-354548	25486	40
Caelo	Chlorhexidine diacetate	15438914	22951SI†	40
Caelo	Chlorhexidine diacetate	21001181	25696SI	50
Caelo	Chlorhexidine diacetate	22000764	26116SI	40
Caelo	Chlorhexidine diacetate	23001289	26832SI	30
Fagron	Chlorhexidine diacetate	15J02-B08-322916	22947SI†	40
Fagron	Chlorhexidine diacetate	18A17-B02-354548	25486SI	40

- 201 609 spectra from a total of 4037 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1149 spectra from 626 *Apo-Ident* customers from 145 batches from the substance/substance group *Chlorhexidine diacetate*.
- Among them are spectra of independent samples from 136 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Chlorhexidine diacetate	19122104	1
	Chlorhexidine diacetate	22003123004	1
	Chlorhexidine diacetate	22003123005	2
	Chlorhexidine diacetate	22003123009	14
	Chlorhexidine diacetate	22003123010	5
	Chlorhexidine diacetate	22003123017	14
	Chlorhexidine diacetate	22C12-B01-223585	2
	Chlorhexidine diacetate	23001289005	2
	Chlorhexidine diacetate	23001289006	2
	Chlorhexidine diacetate	23001289008	4
	Chlorhexidine diacetate	2300129800	1
	Chlorhexidine diacetate	23003317002	1
AEP	Chlorhexidine diacetate	200004515004	1
AEP	Chlorhexidine diacetate	20004515004	1
AHD	Chlorhexidine diacetate	17185812	1
AHD	Chlorhexidine diacetate	22003123017	1
AHD	Chlorhexidine diacetate	23001289006	2
AHL	Chlorhexidine diacetate	15438903	1
Alliance Healthcare	Chlorhexidine diacetate	12177510	1
Alliance	Chlorhexidine diacetate	22003123005	1
Anzag	Chlorhexidine diacetate	12177505	1
Anzag	Chlorhexidine diacetate	18072404	1
Anzag	Chlorhexidine diacetate	70558377	1
Bomastus / Alliance ...	Chlorhexidine diacetate	17185804	1
Caelo	Chlorhexidine diacetate	10154407	1
Caelo	Chlorhexidine diacetate	10154417	1
Caelo	Chlorhexidine diacetate	10154421	1
Caelo	Chlorhexidine diacetate	10154424	1
Caelo	Chlorhexidine diacetate	10154429	1
Caelo	Chlorhexidine diacetate	10154430	2
Caelo	Chlorhexidine diacetate	1072015C	1
Caelo	Chlorhexidine diacetate	11204401	3
Caelo	Chlorhexidine diacetate	11204402	1
Caelo	Chlorhexidine diacetate	11204405	1
Caelo	Chlorhexidine diacetate	11204406	2
Caelo	Chlorhexidine diacetate	11204407	1
Caelo	Chlorhexidine diacetate	11204408	2
Caelo	Chlorhexidine diacetate	12142702	2
Caelo	Chlorhexidine diacetate	12142704	6
Caelo	Chlorhexidine diacetate	12142704ok	1
Caelo	Chlorhexidine diacetate	12142705	3
Caelo	Chlorhexidine diacetate	12142709	1
Caelo	Chlorhexidine diacetate	12142715	4

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Chlorhexidine diacetate	12142720	10
Caelo	Chlorhexidine diacetate	12142725	6
Caelo	Chlorhexidine diacetate	12142726	9
Caelo	Chlorhexidine diacetate	12142727	10
Caelo	Chlorhexidine diacetate	12142734	13
Caelo	Chlorhexidine diacetate	12177502	1
Caelo	Chlorhexidine diacetate	12177503	2
Caelo	Chlorhexidine diacetate	12177504	1
Caelo	Chlorhexidine diacetate	12177505	3
Caelo	Chlorhexidine diacetate	12177510	8
Caelo	Chlorhexidine diacetate	123456	1
Caelo	Chlorhexidine diacetate	1242720	1
Caelo	Chlorhexidine diacetate	1317021	1
Caelo	Chlorhexidine diacetate	13177001	6
Caelo	Chlorhexidine diacetate	13177002	12
Caelo	Chlorhexidine diacetate	13177007	20
Caelo	Chlorhexidine diacetate	13177008	4
Caelo	Chlorhexidine diacetate	13177009	1
Caelo	Chlorhexidine diacetate	13177021	15
Caelo	Chlorhexidine diacetate	13177022	1
Caelo	Chlorhexidine diacetate	13177024	7
Caelo	Chlorhexidine diacetate	15261003	7
Caelo	Chlorhexidine diacetate	15261004	2
Caelo	Chlorhexidine diacetate	15261005	7
Caelo	Chlorhexidine diacetate	15261007	19
Caelo	Chlorhexidine diacetate	15261009	15
Caelo	Chlorhexidine diacetate	15261011	1
Caelo	Chlorhexidine diacetate	15261012	10
Caelo	Chlorhexidine diacetate	15261014	27
Caelo	Chlorhexidine diacetate	15438902	9
Caelo	Chlorhexidine diacetate	15438903	11
Caelo	Chlorhexidine diacetate	15438909	5
Caelo	Chlorhexidine diacetate	15438911	18
Caelo	Chlorhexidine diacetate	15438913	1
Caelo	Chlorhexidine diacetate	15438914	7
Caelo	Chlorhexidine diacetate	15438917	12
Caelo	Chlorhexidine diacetate	1543909	1
Caelo	Chlorhexidine diacetate	15J02-B08-322916	1
Caelo	Chlorhexidine diacetate	160912CH	1
Caelo	Chlorhexidine diacetate	17185802	3
Caelo	Chlorhexidine diacetate	17185803	6
Caelo	Chlorhexidine diacetate	17185804	29
Caelo	Chlorhexidine diacetate	17185805	6
Caelo	Chlorhexidine diacetate	17185807	22
Caelo	Chlorhexidine diacetate	17185808	20
Caelo	Chlorhexidine diacetate	17185810	29
Caelo	Chlorhexidine diacetate	17185811	24
Caelo	Chlorhexidine diacetate	17185812	24
Caelo	Chlorhexidine diacetate	17188504	1
Caelo	Chlorhexidine diacetate	17325801	8
Caelo	Chlorhexidine diacetate	17325803	32
Caelo	Chlorhexidine diacetate	17325808	13
Caelo	Chlorhexidine diacetate	17325809	33
Caelo	Chlorhexidine diacetate	17326809	1
Caelo	Chlorhexidine diacetate	1735801	1
Caelo	Chlorhexidine diacetate	1735803	1
Caelo	Chlorhexidine diacetate	1735809	1
Caelo	Chlorhexidine diacetate	1785808	1
Caelo	Chlorhexidine diacetate	180130CA/17185804	1
Caelo	Chlorhexidine diacetate	18072403	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Chlorhexidine diacetate	18072404	21
Caelo	Chlorhexidine diacetate	1907502	1
Caelo	Chlorhexidine diacetate	190975001	22
Caelo	Chlorhexidine diacetate	19097501	17
Caelo	Chlorhexidine diacetate	19097502	33
Caelo	Chlorhexidine diacetate	19121804	1
Caelo	Chlorhexidine diacetate	191221001	11
Caelo	Chlorhexidine diacetate	191221004	6
Caelo	Chlorhexidine diacetate	19122103	4
Caelo	Chlorhexidine diacetate	19122104	37
Caelo	Chlorhexidine diacetate	200004515003	1
Caelo	Chlorhexidine diacetate	20004515003	11
Caelo	Chlorhexidine diacetate	20004515004	33
Caelo	Chlorhexidine diacetate	20004515005	1
Caelo	Chlorhexidine diacetate	20004515006	14
Caelo	Chlorhexidine diacetate	20004515007	7
Caelo	Chlorhexidine diacetate	2004515006	1
Caelo	Chlorhexidine diacetate	2195172	1
Caelo	Chlorhexidine diacetate	2195195	1
Caelo	Chlorhexidine diacetate	22003123004	10
Caelo	Chlorhexidine diacetate	22003123005	10
Caelo	Chlorhexidine diacetate	22003123006	1
Caelo	Chlorhexidine diacetate	22003123009	5
Caelo	Chlorhexidine diacetate	22003123010	3
Caelo	Chlorhexidine diacetate	22003123017	1
Caelo	Chlorhexidine diacetate	22C12-B01-223585	1
Caelo	Chlorhexidine diacetate	23001289008	1
Caelo	Chlorhexidine diacetate	23012015D	1
Caelo	Chlorhexidine diacetate	31032014B	1
Caelo	Chlorhexidine diacetate	433218072404	1
Caelo	Chlorhexidine diacetate	70558377	1
Caelo	Chlorhexidine diacetate	9(191221004)	1
Caelo	Chlorhexidine diacetate	9113903	1
Caelo	Chlorhexidine diacetate	9113904	2
Caelo	Chlorhexidine diacetate	91139389	1
Caelo	Chlorhexidine diacetate	AK31122020	1
Caeol/ Noweda	Chlorhexidine diacetate	15438911	1
Caeol/Noweda	Chlorhexidine diacetate	19097502	2
Caesar & Loretz GmbH...	Chlorhexidine diacetate	18072404	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	19122104	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	15261012	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	18072403	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	220031263004	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	12142720	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	17185812	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	22003123005	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	20004515003	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	22003123009	2
Caesar & Loretz GmbH...	Chlorhexidine diacetate	19097501	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	19122103	2
Caesar & Loretz GmbH...	Chlorhexidine diacetate	19122104	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	22003123008	1
Caesar & Loretz GmbH/AHD	Chlorhexidine diacetate	22003123004	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	22003123009	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	19122104	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	20004515004	1
Caesar & Loretz GmbH/Gehe	Chlorhexidine diacetate	17185810	1
Caesar & Loretz GmbH/Gehe	Chlorhexidine diacetate	18072404	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	20004515003	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	22003123010	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Chlorhexidine diacetate	19122104	1
Caesar & Loretz GmbH/Otto	Chlorhexidine diacetate	19097502	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	20004515004	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	22003123010	2
Caesar & Loretz GmbH...	Chlorhexidine diacetate	190975001	3
Caesar & Loretz GmbH...	Chlorhexidine diacetate	191221001	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	20004515004	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	22003123004	1
Caesar & Loretz GmbH...	Chlorhexidine diacetate	19122104	1
Caesar & Loretz GmbH	Chlorhexidine diacetate	17185802	1
Caesar & Loretz GmbH	Chlorhexidine diacetate	17185812	2
Caesar & Loretz GmbH	Chlorhexidine diacetate	17325808	5
Caesar & Loretz GmbH	Chlorhexidine diacetate	17325809	2
Caesar & Loretz GmbH	Chlorhexidine diacetate	18072403	1
Caesar & Loretz GmbH	Chlorhexidine diacetate	18072404	7
Caesar & Loretz GmbH	Chlorhexidine diacetate	190975001	2
Caesar & Loretz GmbH	Chlorhexidine diacetate	19097501	3
Caesar & Loretz GmbH	Chlorhexidine diacetate	19097502	8
Caesar & Loretz GmbH	Chlorhexidine diacetate	191221001	11
Caesar & Loretz GmbH	Chlorhexidine diacetate	191221004	1
Caesar & Loretz GmbH	Chlorhexidine diacetate	19122103	1
Caesar & Loretz GmbH	Chlorhexidine diacetate	19122104	10
Caesar & Loretz GmbH	Chlorhexidine diacetate	20004515003	6
Caesar & Loretz GmbH	Chlorhexidine diacetate	20004515004	12
Caesar & Loretz GmbH	Chlorhexidine diacetate	20004515007	1
Caesar & Loretz GmbH	Chlorhexidine diacetate	22003123004	2
Caesar & Loretz GmbH	Chlorhexidine diacetate	22003123005	7
Caesar & Loretz GmbH	Chlorhexidine diacetate	22003123009	7
Caesar & Loretz GmbH	Chlorhexidine diacetate	22003123010	2
Caesar & Loretz GmbH	Chlorhexidine diacetate	22003123017	2
Caesar & Loretz GmbH	Chlorhexidine diacetate	2203123004	1
Caesar & Loretz/Geil...	Chlorhexidine diacetate	19097502	1
Caesar&loretz,Anzag	Chlorhexidine diacetate	12142704	1
caesar	Chlorhexidine diacetate	15261014	1
Cealo/Phoenix	Chlorhexidine diacetate	22003123005	1
Cealo	Chlorhexidine diacetate	13177002	2
cealo	Chlorhexidine diacetate	17185804	1
Cealo	Chlorhexidine diacetate	17325803	1
Ceasar & Loretz GmbH	Chlorhexidine diacetate	80104278	1
Cordes/Noweda	Chlorhexidine diacetate	15438914	1
Euro OTC	Chlorhexidine diacetate	10154430	1
Euro OTC	Chlorhexidine diacetate	15261004	1
Euro OTC	Chlorhexidine diacetate	17185810	3
Euro OTC	Chlorhexidine diacetate	17325809	1
Euro OTC	Chlorhexidine diacetate	1785805	1
Fagron	Chlorhexidine diacetate	12E14-N11	1
Fagron	Chlorhexidine diacetate	13177008	1
Fagron	Chlorhexidine diacetate	13E03-B06	1
Fagron	Chlorhexidine diacetate	13E03-B06-287926	2
Fagron	Chlorhexidine diacetate	13E03-B06-287929	1
Fagron	Chlorhexidine diacetate	15261009	1
Fagron	Chlorhexidine diacetate	15438901	1
Fagron	Chlorhexidine diacetate	15J02-B08	2
Fagron	Chlorhexidine diacetate	15J02-B08-322916	2
Fagron	Chlorhexidine diacetate	17185811	1
Fagron	Chlorhexidine diacetate	17325801	1
Fagron	Chlorhexidine diacetate	17D25-B04-339937	3
Fagron	Chlorhexidine diacetate	1-8991-1-01-01	1
Fagron	Chlorhexidine diacetate	19F27-B03-364809	1
Fagron	Chlorhexidine diacetate	22C12-B01-223585	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Chlorhexidine diacetate	A-130037	1
Fagron	Chlorhexidine diacetate	A-170073	1
Fiebig	Chlorhexidine diacetate	15261014	1
Fiebig	Chlorhexidine diacetate	17185807	1
Fiebig	Chlorhexidine diacetate	17325803	1
GEHE	Chlorhexidine diacetate	12142734	1
Gehe	Chlorhexidine diacetate	15261007	1
Gehe	Chlorhexidine diacetate	15261009	2
Gehe	Chlorhexidine diacetate	15438909	1
Gehe	Chlorhexidine diacetate	17185804	1
Gehe	Chlorhexidine diacetate	17185805	1
Gehe	Chlorhexidine diacetate	17325803	1
Gehe	Chlorhexidine diacetate	22003123009	2
Gehe	Chlorhexidine diacetate	22003123017	1
Jenne	Chlorhexidine diacetate	17185808	1
Jenne	Chlorhexidine diacetate	17185810	1
Jenne	Chlorhexidine diacetate	22003123010	1
Kehr	Chlorhexidine diacetate	22003123017	1
keine Angabe	Chlorhexidine diacetate	11204402	2
Medichem S.A. ES/Noweda	Chlorhexidine diacetate	13177007	1
Nachprüfung	Chlorhexidine diacetate	2082019-9	1
Noweda	Chlorhexidine diacetate	12142720	1
Noweda	Chlorhexidine diacetate	12142727	1
Noweda	Chlorhexidine diacetate	15438911	2
Noweda	Chlorhexidine diacetate	17185804	1
Noweda	Chlorhexidine diacetate	17185805	1
Noweda	Chlorhexidine diacetate	17185808	1
Noweda	Chlorhexidine diacetate	17185811	1
Noweda	Chlorhexidine diacetate	17325808	2
Noweda	Chlorhexidine diacetate	1785803	1
Noweda	Chlorhexidine diacetate	19097501	1
Noweda	Chlorhexidine diacetate	22003123009	2
Phoenix	Chlorhexidine diacetate	11204408	1
Phoenix	Chlorhexidine diacetate	12142726	1
Phoenix	Chlorhexidine diacetate	12142734	1
Phoenix	Chlorhexidine diacetate	13177002	1
Phoenix	Chlorhexidine diacetate	15438917	1
Phoenix	Chlorhexidine diacetate	191221000	1
phönix	Chlorhexidine diacetate		1
phönix	Chlorhexidine diacetate	15438911	1
Phönix	Chlorhexidine diacetate	15438917	1
Phönix	Chlorhexidine diacetate	15J02-B08-322916	1
Phönix	Chlorhexidine diacetate	17185803	1
Phönix	Chlorhexidine diacetate	17185804	1
Phönix	Chlorhexidine diacetate	17325803	1
Phönix	Chlorhexidine diacetate	17325809	2
phönix	Chlorhexidine diacetate	19122104	1
Phönix	Chlorhexidine diacetate	22003123004	1
Phönix	Chlorhexidine diacetate	22003123009	1
Phönix	Chlorhexidine diacetate	9113916	2
Phönix	Chlorhexidine diacetate	Retest09113916	1
Sanacorp 107	Chlorhexidine diacetate	190975001	1
Sanacorp	Chlorhexidine diacetate		1
Sanacorp	Chlorhexidine diacetate	12142734	1
Sanacorp	Chlorhexidine diacetate	17185804	1
Sanacorp	Chlorhexidine diacetate	18072403	1
SANACORP	Chlorhexidine diacetate	19097502	1
Sanacorp	Chlorhexidine diacetate	191221004	1
Sanacorp	Chlorhexidine diacetate	22003123009	1
Sanacorp	Chlorhexidine diacetate	22003123017	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Chlorhexidine diacetate	7/AKD6	1
Shaanxi dasehng Phar…	Chlorhexidine diacetate	19122104	1
Shaanxi Dasheng Phar…	Chlorhexidine diacetate	17185807	1
Shaanxi/Phoenix	Chlorhexidine diacetate	CAB-180103	1
Wepa/Wepa	Chlorhexidine diacetate	15438902	1

- 234 918 spectra from 1515 *Apo-Ident* customers from a total of 49 115 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Chlorhexidine diacetate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Chlorhexidine diacetate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	840	0	152 122
Type B	0	475	0	201 609
Type C	0	1135	14	234 918

The substance/substance group *Chlorhexidine diacetate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.2857 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.7368 %)
Type C	100.0000 % (> 99.9007 %)	98.7815 % (> 98.5205 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20989	20989	0.00	179.91
21041	20989	18.34	179.86
22280	22456	5.53	184.08
22456	22456	0.00	181.39
22900	22900	0.00	183.51
22946	23044	5.97	182.14
22947	22456	5.77	181.23
22951	22900	6.07	183.61
23041	23041	0.00	183.30
23042	23042	0.00	183.68
23043	23043	0.00	184.10
23044	23044	0.00	183.33
23048	23048	0.00	182.48
26456	22456	5.31	183.62
26483	26483	0.00	180.99
26816	20989	51.57	177.90

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Chlorocresol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20185-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Chlorocresol; Chlorocresolum

Special notes

When selecting the *Chlorocresol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Chlorocresol	5	2	16

Second-stage model

For differentiation of the substance/substance group *Chlorocresol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Chlorocresol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	89.04	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Chlorocresol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Chlorocresol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Chlorocresol	13275106	21512	60	20130828
Caelo	Chlorocresol	13275106	21513	60	20130828
Caelo	Chlorocresol	163378	23357	40	20170124*
Caelo	Chlorocresol	182523	24406	40	20180919*
Caelo	Chlorocresol	190837	24717	40	20190508*
Caelo	Chlorocresol	21004157	27127	40	20220303*
Caelo	Chlorocresol	21004157	27127SI	20	20220303*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 300 spectra of 7 reference samples from the substance/substance group *Chlorocresol*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 662 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Chlorocresol*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Chlorocresol	15114107	23411	40
Caelo	Chlorocresol	181360	24050	40

- 202 004 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 36 spectra from 27 *Apo-Ident* customers from 16 batches from the substance/substance group *Chlorocresol*.

- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Chlorocresol	22002861005	1
Caelo	Chlorocresol	10145239	3
Caelo	Chlorocresol	12111013	2
Caelo	Chlorocresol	12111017	2
Caelo	Chlorocresol	13275117	1
Caelo	Chlorocresol	15114107	1
Caelo	Chlorocresol	18027101	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Chlorocresol	18027110	2
Caelo	Chlorocresol	18136006	6
Caelo	Chlorocresol	20004363020	1
Caelo	Chlorocresol	20101808	1
Caelo	Chlorocresol	2041513	1
Caelo	Chlorocresol	23415422	1
Caelo	Chlorocresol	4613M-01260	1
Caelo	Chlorocresol	7061304	1
Caesar & Loretz GmbH/Gehe	Chlorocresol	18136006	1
Caesar & Loretz GmbH…	Chlorocresol	18027101	1
Caesar & Loretz GmbH	Chlorocresol	12111017	1
Caesar & Loretz GmbH	Chlorocresol	18136006	2
Noweda	Chlorocresol	12111017	1
Noweda	Chlorocresol	22002861005	1
Spangropharm	Chlorocresol		1

- 236 031 spectra from 1515 *Apo-Ident* customers from a total of 49 242 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Chlorocresol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Chlorocresol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	80	0	202 004
Type C	0	36	0	236 031

The substance/substance group *Chlorocresol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 83.3333 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21512	24406	15.85	163.94
21513	27127	12.60	167.64
23357	23357	0.00	153.35
24406	24406	0.00	170.49
24717	24717	0.00	156.17
27127	27127	0.00	168.10

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Chlorprothixene hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	24105-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Chlorprothixene hydrochloride; Chlorprothixeni hydrochloridum

Special notes

When selecting the *Chlorprothixene hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Chlorprothixene hydrochloride	2	1	0

Second-stage model

For differentiation of the substance/substance group *Chlorprothixene hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Chlorprothixene hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Doxepin hydrochloride	35.76	–
Benzydamine hydrochloride	131.27	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Chlorprothixene hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Chlorprothixene hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Chlorprothixene hydrochloride	AP05061117C	24105	40	1810394
Euro OTC	Chlorprothixene hydrochloride	2003005	25290	40	20200728*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Chlorprothixene hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 882 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Chlorprothixene hydrochloride*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Audor Pharma	Chlorprothixene hydrochloride	AP04120418C	24434	40

- 202 044 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Chlorprothixene hydrochloride*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Chlorprothixene hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Chlorprothixene hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or

incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	80	0	152 882
Type B	0	40	0	202 044
Type C	0	0	0	236 067

The substance/substance group *Chlorprothixene hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24105	24105	0.00	61.52
25290	25290	0.00	62.24

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Chlortetracycline hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20845-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Chlortetracycline hydrochloride; Chlortetracyclini hydrochloridum

Special notes

When selecting the *Chlortetracycline hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Chlortetracycline hydrochloride	7	4	89

Second-stage model

For differentiation of the substance/substance group *Chlortetracycline hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Chlortetracycline hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Tetracycline hydrochloride	57.52	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Chlortetracycline hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Chlortetracycline hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Chlortetracycline hydroch…	1108051-02	21241	40	20111013
Euro OTC	Chlortetracycline hydroch…	1604015	22541	40	20160510*
Euro OTC	Chlortetracycline hydroch…	1910002	24959	40	20191107*
Euro OTC	Chlortetracycline hydroch…	2009026	25573	40	20210104*
Euro OTC	Chlortetracycline hydroch…	2205011	26229	40	20220704*
Fagron	Chlortetracycline hydroch…	12K30-N07	20845	40	1405318
Fagron	Chlortetracycline hydroch…	12K30-N07	21222	40	20121210
Fagron	Chlortetracycline hydroch…	14J08-B07-307742	21877	60	20141029

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 340 spectra of 8 reference samples from the substance/substance group *Chlortetracycline - hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 622 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 6 reference samples from the substance/substance group *Chlortetracycline - hydrochloride*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Chlortetracycline hydroch…	1604015-01	22975	40
Euro OTC	Chlortetracycline hydroch…	1803037	24092	40
Euro OTC	Chlortetracycline hydroch…	2402024	27365	40
Fagron	Chlortetracycline hydroch…	16B10-B09-329778	23571	30
Euro OTC	Chlortetracycline hydroch…	2205011	26229SI†	20
Euro OTC	Chlortetracycline hydroch…	2402024	27365SI	20

- 201 894 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 673 spectra from 302 *Apo-Ident* customers from 102 batches from the substance/substance group *Chlortetracycline hydrochloride*.

- Among them are spectra of independent samples from 88 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Chlortetracycline hydroch…	2009026-01	2
	Chlortetracycline hydroch…	2205011-01	5
AHD/Euro	Chlortetracycline hydroch…	1803037	2
ALH	Chlortetracycline hydroch…	16B10-B09-320304	1
Alliance Healthcare	Chlortetracycline hydroch…	12K30-N07	1
Anzag/ Euro OT	Chlortetracycline hydroch…	1803037-02	1
Anzag: 07.09.12 ek:4.01	Chlortetracycline hydroch…	12C16-N01	1
Anzag	Chlortetracycline hydroch…	1604015-01	1
apo-ident	Chlortetracycline hydroch…	1803037-01	2
apomix	Chlortetracycline hydroch…	2009026-01	1
Caelo	Chlortetracycline hydroch…		1
Caelo	Chlortetracycline hydroch…	1412008-01	1
Caelo	Chlortetracycline hydroch…	141200802	1
Caelo	Chlortetracycline hydroch…	1412008-02	1
Caelo	Chlortetracycline hydroch…	141200803	1
Caelo	Chlortetracycline hydroch…	142008-03	1
Caelo	Chlortetracycline hydroch…	14J08-B07-300249	1
Caelo	Chlortetracycline hydroch…	14J08-B07-303352	1
Caelo	Chlortetracycline hydroch…	14j08-b07-307100	1
Caelo	Chlortetracycline hydroch…	1604015-01	4
Caelo	Chlortetracycline hydroch…	1604015-61	1
Caelo	Chlortetracycline hydroch…	16B10-B09-318088	1
Caelo	Chlortetracycline hydroch…	16B10-B09-322716	1
Caelo	Chlortetracycline hydroch…	16B10B09329778	1
Caelo	Chlortetracycline hydroch…	16B10-B09-336332	1
Caelo	Chlortetracycline hydroch…	16B10-B09-347439	3
Caelo	Chlortetracycline hydroch…	1803037-01	3
Caelo	Chlortetracycline hydroch…	1803037-03	1
Caelo	Chlortetracycline hydroch…	1803038-01	1
Caelo	Chlortetracycline hydroch…	1910002-01	1
Caelo	Chlortetracycline hydroch…	191002-02	1
Caelo	Chlortetracycline hydroch…	FC13030134	1
Caelo	Chlortetracycline hydroch…	FC15100204	1
Caesar & Loretz GmbH	Chlortetracycline hydroch…	12C16-N01	1
EuRho/ AHD	Chlortetracycline hydroch…	1803037-01	5
EuRho/ NOWEDA	Chlortetracycline hydroch…	1803037-02	1
Eurho/Fiebig	Chlortetracycline hydroch…	1910002-01	1
EuRho/Gehe	Chlortetracycline hydroch…	1803037	1
EuRho/Gehe	Chlortetracycline hydroch…	2009026-01	1
Eurho/Phönix	Chlortetracycline hydroch…	220501101	1
EuRho	Chlortetracycline hydroch…	1412008-02	1
EuRho	Chlortetracycline hydroch…	1803037-01	1
EuRho	Chlortetracycline hydroch…	1910002-01	2
Euro OTC	Chlortetracycline hydroch…		1
Euro OTC	Chlortetracycline hydroch…	10I29-N04	1
Euro OTC	Chlortetracycline hydroch…	1108051-01	8
Euro OTC	Chlortetracycline hydroch…	110805102	1
Euro OTC	Chlortetracycline hydroch…	1108051-02	7
Euro OTC	Chlortetracycline hydroch…	1412008/03	1
Euro OTC	Chlortetracycline hydroch…	1412008-01	9
Euro OTC	Chlortetracycline hydroch…	141200802	2
Euro OTC	Chlortetracycline hydroch…	1412008-02	15
Euro OTC	Chlortetracycline hydroch…	141200803	1
Euro OTC	Chlortetracycline hydroch…	1412008-03	5
Euro OTC	Chlortetracycline hydroch…	16004015-15	1
Euro OTC	Chlortetracycline hydroch…	160401501	2
Euro OTC	Chlortetracycline hydroch…	1604015-01	63
Euro OTC	Chlortetracycline hydroch…	160401502	1
Euro OTC	Chlortetracycline hydroch…	1604015-02	3
Euro OTC	Chlortetracycline hydroch…	16b10-b09-326865	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Chlortetracycline hydroch…	16B10-B09-348359	1
Euro OTC	Chlortetracycline hydroch…	16B10-B09-352970	1
Euro OTC	Chlortetracycline hydroch…	1803037	2
Euro OTC	Chlortetracycline hydroch…	1803037_01	4
Euro OTC	Chlortetracycline hydroch…	180303701	1
Euro OTC	Chlortetracycline hydroch…	1803037-01	61
Euro OTC	Chlortetracycline hydroch…	1803037-02	3
Euro OTC	Chlortetracycline hydroch…	1803037-03	22
Euro OTC	Chlortetracycline hydroch…	190002-02	1
Euro OTC	Chlortetracycline hydroch…	19100002-02	1
Euro OTC	Chlortetracycline hydroch…	1910002	1
Euro OTC	Chlortetracycline hydroch…	191000201	1
Euro OTC	Chlortetracycline hydroch…	1910002-01	85
Euro OTC	Chlortetracycline hydroch…	1910002-02	26
Euro OTC	Chlortetracycline hydroch…	191002-01	2
Euro OTC	Chlortetracycline hydroch…	200902601	1
Euro OTC	Chlortetracycline hydroch…	2009026-01	59
Euro OTC	Chlortetracycline hydroch…	2009026-02	2
Euro OTC	Chlortetracycline hydroch…	2205011-01	1
Euro OTC	Chlortetracycline hydroch…	2901009V-03	1
Euro OTC	Chlortetracycline hydroch…	4612Q-01155	1
Euro OTC	Chlortetracycline hydroch…	4931439	1
Euro OTC	Chlortetracycline hydroch…	5113I01155	1
Euro OTC	Chlortetracycline hydroch…	700156	1
Euro OTC	Chlortetracycline hydroch…	80218-A	1
Euro OTC	Chlortetracycline hydroch…	FC15110253	1
Euro OTC	Chlortetracycline hydroch…	FC21020106	1
EURO Pharma	Chlortetracycline hydroch…	1108051-01	1
EUro/AHD	Chlortetracycline hydroch…	1108051-02	1
euro/gehe	Chlortetracycline hydroch…	1604015-01	1
Euro/Noweda	Chlortetracycline hydroch…	1604015-01	1
EuRo/Phönix	Chlortetracycline hydroch…	160401501	1
Euro/Phönix	Chlortetracycline hydroch…	2009026-01	2
Euro	Chlortetracycline hydroch…	1108051-02	1
Fagron	Chlortetracycline hydroch…		1
Fagron	Chlortetracycline hydroch…	12C16-N01	1
Fagron	Chlortetracycline hydroch…	12H28N09	1
Fagron	Chlortetracycline hydroch…	12H28-N09	4
Fagron	Chlortetracycline hydroch…	12k30-N07	1
Fagron	Chlortetracycline hydroch…	12K30-N07	9
Fagron	Chlortetracycline hydroch…	13/11-N07	4
Fagron	Chlortetracycline hydroch…	13K26-N06	2
Fagron	Chlortetracycline hydroch…	13l11-N07	1
Fagron	Chlortetracycline hydroch…	14J08-B07	4
Fagron	Chlortetracycline hydroch…	14J08-B07-300247	2
Fagron	Chlortetracycline hydroch…	14J08-B07-300250	8
Fagron	Chlortetracycline hydroch…	14J08-B07-303350	1
Fagron	Chlortetracycline hydroch…	14J08-B07-303352	7
Fagron	Chlortetracycline hydroch…	14J08B07307100	3
Fagron	Chlortetracycline hydroch…	14J08-B07-307100	7
Fagron	Chlortetracycline hydroch…	14J08-B07-307742	4
Fagron	Chlortetracycline hydroch…	16b10-b09	1
Fagron	Chlortetracycline hydroch…	16B10-B09	7
Fagron	Chlortetracycline hydroch…	16B10-B09-318088	5
Fagron	Chlortetracycline hydroch…	16B10-B09-320304	6
Fagron	Chlortetracycline hydroch…	16B10-B09-322715	5
Fagron	Chlortetracycline hydroch…	16B10-B09-322716	2
Fagron	Chlortetracycline hydroch…	16B10-B09-326865	1
Fagron	Chlortetracycline hydroch…	16B10-B09-329778	2
Fagron	Chlortetracycline hydroch…	16B10-B09-331443	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Chlortetracycline hydroch…	16b10-b09-336332	1
Fagron	Chlortetracycline hydroch…	16B10-B09-336332	10
Fagron	Chlortetracycline hydroch…	16B10-B09-342410	2
Fagron	Chlortetracycline hydroch…	16b10b09347439	1
Fagron	Chlortetracycline hydroch…	16B10-B09-348359	1
Fagron	Chlortetracycline hydroch…	16B10-B09-351565	4
Fagron	Chlortetracycline hydroch…	16B10-B09-352970	6
Fagron	Chlortetracycline hydroch…	16b10b09355611	1
Fagron	Chlortetracycline hydroch…	1803037-01	2
Fagron	Chlortetracycline hydroch…	1803037-03	2
Fagron	Chlortetracycline hydroch…	1910002-01	2
Fagron	Chlortetracycline hydroch…	191002-01	1
Fagron	Chlortetracycline hydroch…	27121306	1
Fagron	Chlortetracycline hydroch…	3918Q-01155	1
Fagron	Chlortetracycline hydroch…	5014M-01155T	1
Fagron	Chlortetracycline hydroch…	700156-B09-347439	1
Fagron	Chlortetracycline hydroch…	FC11051038	1
Fagron	Chlortetracycline hydroch…	FC13030134	1
Fagron	Chlortetracycline hydroch…	FC15100204	5
Fiebig/EuRho	Chlortetracycline hydroch…	1910002-01	1
Fiebig	Chlortetracycline hydroch…	1412008-01	1
Fiebig	Chlortetracycline hydroch…	1604015-01	1
Fiebig	Chlortetracycline hydroch…	1910002-02	2
Fiebig	Chlortetracycline hydroch…	FC15100204	1
Fragon/Sanacorp	Chlortetracycline hydroch…	16B10-B09-352970	1
Fuijan/Noweda	Chlortetracycline hydroch…	FC17090368	1
Fuijan/Noweda	Chlortetracycline hydroch…	FC19040113	2
Fujan Pharmaceutic	Chlortetracycline hydroch…	2009026-01	3
Fujang Fukang China	Chlortetracycline hydroch…	200902601	1
Fujian Fukang Phamaceutic	Chlortetracycline hydroch…	2205011-01	1
Fujian Fukang/Phoenix	Chlortetracycline hydroch…	2009026-01	3
Gehe/Fagro	Chlortetracycline hydroch…	16B10-B09-338800	1
GEHE	Chlortetracycline hydroch…	1604015-01	1
Gehe	Chlortetracycline hydroch…	16B10-B09	2
Gehe	Chlortetracycline hydroch…	16B10-B09-322715	1
Gehe	Chlortetracycline hydroch…	16B10-B09-322716	1
Gehe	Chlortetracycline hydroch…	1910002-02	1
Gehe	Chlortetracycline hydroch…	2205011-01	1
Geibo/Euro11.06.19	Chlortetracycline hydroch…	1803037-01	1
Krieger	Chlortetracycline hydroch…	12C16-No1	1
Nachprüfung 2574	Chlortetracycline hydroch…	1108051-01	1
Nachprüfung	Chlortetracycline hydroch…	1108051-01	1
Noweda	Chlortetracycline hydroch…	12c16-n01	1
Noweda	Chlortetracycline hydroch…	1412008-01	1
Noweda	Chlortetracycline hydroch…	160401501	1
Noweda	Chlortetracycline hydroch…	1803037	1
Noweda	Chlortetracycline hydroch…	1803037-01	1
Noweda	Chlortetracycline hydroch…	1910002-02	2
Noweda	Chlortetracycline hydroch…	2205011-01	1
Noweda	Chlortetracycline hydroch…	EurootcPharama	1
Noweda	Chlortetracycline hydroch…	EuroOTCPharma	1
Phoenix	Chlortetracycline hydroch…	110805102	1
Phoenix	Chlortetracycline hydroch…	16B10-B09-322716	1
Phoenix	Chlortetracycline hydroch…	1803037-01	1
Phoenix	Chlortetracycline hydroch…	3407	1
Phönix/apo ident	Chlortetracycline hydroch…	1604015-01	1
Phönix/EurHo	Chlortetracycline hydroch…	1803037-01	1
Phönix/EurHo	Chlortetracycline hydroch…	191000201	1
Phönix/Euro	Chlortetracycline hydroch…	180303701	2
Phönix/EuRo	Chlortetracycline hydroch…	1910002-02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Chlortetracycline hydroch…	1108051-02	2
Phönix	Chlortetracycline hydroch…	1412008-01	1
phönix	Chlortetracycline hydroch…	16B10-B09-336332	1
Phönix	Chlortetracycline hydroch…	1803037	1
Phönix	Chlortetracycline hydroch…	1803037-03	1
Phönix	Chlortetracycline hydroch…	FC17090368	1
Sanacop	Chlortetracycline hydroch…	1412008-02	1
Sanacorp	Chlortetracycline hydroch…	1108051-01	1
Sanacorp	Chlortetracycline hydroch…	14J08-B07	1
Sanacorp	Chlortetracycline hydroch…	1604015-01	1
Sanacorp	Chlortetracycline hydroch…	16B10-B09	1
Sanacorp	Chlortetracycline hydroch…	180303701	1
Sanacorp	Chlortetracycline hydroch…	FC15100204	1

- 235 394 spectra from 1515 *Apo-Ident* customers from a total of 49 157 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Chlortetracycline hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Chlortetracycline hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	340	0	152 622
Type B	0	190	0	201 894
Type C	0	662	11	235 394

The substance/substance group *Chlortetracycline hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2353 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9007 %)	98.3655 % (> 97.9198 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested

reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20845	20845	0.00	57.99
21222	20845	7.52	60.42
21241	20845	10.13	57.83
21877	22541	10.13	65.59
22541	22541	0.00	61.57
24959	24959	0.00	87.65
25573	25573	0.00	76.82
26229	26229	0.00	59.21

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cholesterol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20446-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cholesterol; Cholesterolum

Special notes

When selecting the *Cholesterol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cholesterol	8	5	176

Second-stage model

For differentiation of the substance/substance group *Cholesterol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cholesterol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Wool alcohols	72.74	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cholesterol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cholesterol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cholesterol	160444	22461	60	20160222*
Caelo	Cholesterol	16044415	23760	40	1804387
Caelo	Cholesterol	21000039004	25517	40	20210127
Caelo	Cholesterol	23002121	26963	40	20230922*
Caelo	Cholesterol	23002121	26963SI	20	20230922*
Fagron	Cholesterol	13F10-B40	21219	40	20131223
Fagron	Cholesterol	15J23-B03-325106	22971	40	20151103
Fagron	Cholesterol	17E17-B05-339074	23937	40	20170620
Fagron	Cholesterol	22D05-B03-220575	26160	40	20220519
Fagron	Cholesterol	22D05-B03-220575	26160SI	20	20220519

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 380 spectra of 10 reference samples from the substance/substance group *Cholesterol*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 582 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 220 spectra of 6 reference samples from the substance/substance group *Cholesterol*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cholesterol	13148703	21310	40
Caelo	Cholesterol	190549	24712	40
Caelo	Cholesterol	22001179	26111	40
Fagron	Cholesterol	16G05-B03-331396	23522	40
Fagron	Cholesterol	24D26-B01-240098	27424	40
Caelo	Cholesterol	22001179	26111SI	20

- 201 864 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 442 spectra from 165 *Apo-Ident* customers from 184 batches from the substance/substance group *Cholesterol*.

- Among them are spectra of independent samples from 175 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cholesterol	22001179013	1
	Cholesterol	2203-B01-229435	1
	Cholesterol	22D05-B03-220341	1
	Cholesterol	22J03-B01	1
	Cholesterol	22j03b01224448	1
	Cholesterol	22j03-b01-224452	1
	Cholesterol	22J03-B01-229435	4
	Cholesterol	23D21-B03-229928	1
	Cholesterol	41172	2
	Cholesterol	B01-2244502	1
	Cholesterol	B01-2386705	2
AHD	Cholesterol	17K16-B11-352718	1
Anzag/Fargon	Cholesterol	19J18-B02	1
Caelo	Cholesterol	11242103	1
Caelo	Cholesterol	12155605	1
Caelo	Cholesterol	12248403	1
Caelo	Cholesterol	13056903	1
Caelo	Cholesterol	13148704	1
Caelo	Cholesterol	14027201	1
Caelo	Cholesterol	14122501	2
Caelo	Cholesterol	14208602	1
Caelo	Cholesterol	15028303	1
Caelo	Cholesterol	15301803	3
Caelo	Cholesterol	15358801	5
Caelo	Cholesterol	15407101	2
Caelo	Cholesterol	15407102	2
Caelo	Cholesterol	15B09-B02-308259	1
Caelo	Cholesterol	15G31-B05-312376	1
Caelo	Cholesterol	15J23-B03	1
Caelo	Cholesterol	15J23-B03_329505	1
Caelo	Cholesterol	16044402	1
Caelo	Cholesterol	16044407	4
Caelo	Cholesterol	16044408	2
Caelo	Cholesterol	16044409	2
Caelo	Cholesterol	16044413	4
Caelo	Cholesterol	16044415	4
Caelo	Cholesterol	16044416	6
Caelo	Cholesterol	16G05-B03	1
Caelo	Cholesterol	17K16-B11-343922	1
Caelo	Cholesterol	17K16-B11-345814	1
Caelo	Cholesterol	17K16-B11-348760	1
Caelo	Cholesterol	17K16-B11-350557	2
Caelo	Cholesterol	18097102	2
Caelo	Cholesterol	18097202	2
Caelo	Cholesterol	19054901	7
Caelo	Cholesterol	19054903	6
Caelo	Cholesterol	191949001	2
Caelo	Cholesterol	191949003	2
Caelo	Cholesterol	19194902	4
Caelo	Cholesterol	19194903	2
Caelo	Cholesterol	19194904	9
Caelo	Cholesterol	19I18-B02	1
Caelo	Cholesterol	19I20-B08	1
Caelo	Cholesterol	19J18-B02-201592	1
Caelo	Cholesterol	19J18-B01-201136	1
Caelo	Cholesterol	20G08-B02	1
Caelo	Cholesterol	20G08-B02-202266	3
Caelo	Cholesterol	21000039004	2
Caelo	Cholesterol	21000039006	4
Caelo	Cholesterol	21000039009	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cholesterol	2100039009	1
Caelo	Cholesterol	21C18-B01-213585	2
Caelo	Cholesterol	21F08-B20-215610	1
Caelo	Cholesterol	22001179004	1
Caelo	Cholesterol	27212	1
Caelo	Cholesterol	32124	1
Caelo	Cholesterol	B02-2015901	1
Caesar & Loretz GmbH	Cholesterol	18097202	1
Caesar & Loretz GmbH	Cholesterol	19194903	2
Ebert-Jacobi	Cholesterol	16044408	1
Euro OTC	Cholesterol	13F10-B40-289016	1
Fagro/EJ	Cholesterol	17K16-B11_348760	1
Fagron	Cholesterol		1
Fagron	Cholesterol	10B15-N07	1
Fagron	Cholesterol	10H24-N06	1
Fagron	Cholesterol	11A17-N07	1
Fagron	Cholesterol	1213585	1
Fagron	Cholesterol	12D02-N10	1
Fagron	Cholesterol	12I13-N02	2
Fagron	Cholesterol	13C25-N12	2
Fagron	Cholesterol	13F10-B40	1
Fagron	Cholesterol	13F10-B40-289016	2
Fagron	Cholesterol	13G10-N11	3
Fagron	Cholesterol	14B27-B05	2
Fagron	Cholesterol	14B27-B05-293548	3
Fagron	Cholesterol	14B27-B05-293550	1
Fagron	Cholesterol	14G04-B02	1
Fagron	Cholesterol	14G04-B02-300830	2
Fagron	Cholesterol	14G04-B02-300831	1
Fagron	Cholesterol	15B09	1
Fagron	Cholesterol	15B09-B02	1
Fagron	Cholesterol	15B09-B02-308259	4
Fagron	Cholesterol	15B09-B02-308847	2
Fagron	Cholesterol	15G31-B05	2
Fagron	Cholesterol	15G31-B05_316721	1
Fagron	Cholesterol	15G31-B05-312377	1
Fagron	Cholesterol	15G31-B05-312378	1
Fagron	Cholesterol	15G31-B05-314182	2
Fagron	Cholesterol	15G31-B05-316721	3
Fagron	Cholesterol	15J23-B03	1
Fagron	Cholesterol	15J23B03320483	1
Fagron	Cholesterol	15J23-B03-320483	5
Fagron	Cholesterol	15J23B03322902	1
Fagron	Cholesterol	15J23-B03-322902	1
Fagron	Cholesterol	15j23-B03-325106	1
Fagron	Cholesterol	15J23B03325106	1
Fagron	Cholesterol	15J23-B03-325106	5
Fagron	Cholesterol	15J23B03328249	1
Fagron	Cholesterol	15J23-B03-328249	2
Fagron	Cholesterol	16G05-B03	1
Fagron	Cholesterol	16G05-B03-331396	2
Fagron	Cholesterol	16G05-B03-331397	1
Fagron	Cholesterol	16G05-B03-333996	3
Fagron	Cholesterol	16G05-B03-334366	1
Fagron	Cholesterol	16GB05-B03	1
Fagron	Cholesterol	17E17-B05	2
Fagron	Cholesterol	17E17-B05-337588	5
Fagron	Cholesterol	17E17-B05-339074	8
Fagron	Cholesterol	17E17-B05-339075	2
Fagron	Cholesterol	17K16-B11-343922	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cholesterol	17K16-B11-343923	1
Fagron	Cholesterol	17K16-B11-345814	2
Fagron	Cholesterol	17K16-B11-348760	4
Fagron	Cholesterol	17K16-B11-348761	3
Fagron	Cholesterol	17K16-B11-348762	1
Fagron	Cholesterol	17K16-B11-349922	1
Fagron	Cholesterol	17K16B11350557	1
Fagron	Cholesterol	17K16-B11-350557	6
Fagron	Cholesterol	17K16-B11-352718	13
Fagron	Cholesterol	17K16-B11-355385	7
Fagron	Cholesterol	17k16-B11-43922	1
Fagron	Cholesterol	18I03-B06	1
Fagron	Cholesterol	18I03-B06-353374	2
Fagron	Cholesterol	18I03-B06-355386	1
Fagron	Cholesterol	18I03-B06-356700	1
Fagron	Cholesterol	18J18-B02-201591	1
Fagron	Cholesterol	19120B08200506	1
Fagron	Cholesterol	19120-B08-200506	2
Fagron	Cholesterol	19120-BO8-200506	1
Fagron	Cholesterol	1920B0B-200561	1
Fagron	Cholesterol	19E20-B02-191413	1
Fagron	Cholesterol	19E20-B02-192819	2
Fagron	Cholesterol	19G12-B0313-194214	1
Fagron	Cholesterol	19g12-b13-194214	1
Fagron	Cholesterol	19G12-B13-194214	8
Fagron	Cholesterol	19G12-B13-194216	1
Fagron	Cholesterol	19I20-B08	2
Fagron	Cholesterol	19I20-B08-196479	4
Fagron	Cholesterol	19I20-B08-196480	1
Fagron	Cholesterol	19I20-B08-200506	6
Fagron	Cholesterol	19I20-B08-200559	2
Fagron	Cholesterol	19I20-B08-200561	4
Fagron	Cholesterol	19J18-B01-201136	5
Fagron	Cholesterol	19J18-B02	1
Fagron	Cholesterol	19J18B02196477	1
Fagron	Cholesterol	19J18-B02-196477	8
Fagron	Cholesterol	19J18-B02-201591	5
Fagron	Cholesterol	19J18-B02-201592	1
Fagron	Cholesterol	19j18-BO2	1
Fagron	Cholesterol	19j18-bo2-201595	1
Fagron	Cholesterol	19J19-B02-201592	1
Fagron	Cholesterol	19l20-B08-196480	1
Fagron	Cholesterol	2013U-01270	1
Fagron	Cholesterol	20F25-B99-201594	3
Fagron	Cholesterol	20G08-0B02-202266	1
Fagron	Cholesterol	20G08-B02	4
Fagron	Cholesterol	20G08-B02-201946	6
Fagron	Cholesterol	20G08-B02-202265	5
Fagron	Cholesterol	20G08-B02-202266	9
Fagron	Cholesterol	20G08-B02-202266	1
Fagron	Cholesterol	20G08-BO2-201946	1
Fagron	Cholesterol	20G08-N02-202265	1
Fagron	Cholesterol	21c18B01213585	1
Fagron	Cholesterol	21C18B01213585	2
Fagron	Cholesterol	21C18-B01-213585	14
Fagron	Cholesterol	21C18-B01-213586	1
Fagron	Cholesterol	21C18-BO1	1
Fagron	Cholesterol	21F08-b20-213589	1
Fagron	Cholesterol	21F08-B20	1
Fagron	Cholesterol	22d05-b03-220495	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cholesterol	22J03-B01-224448	2
Fagron	Cholesterol	27212	1
Fagron	Cholesterol	2OG08-B02-202266	1
Fagron	Cholesterol	30197	1
Fagron	Cholesterol	30969	2
Fagron	Cholesterol	31941	2
Fagron	Cholesterol	322124	1
Fagron	Cholesterol	34342	4
Fagron	Cholesterol	36062	2
Fagron	Cholesterol	8J28-N10	1
Fagron	Cholesterol	B01-2011306	1
Fagron	Cholesterol	B02_2022606	1
Fagron	Cholesterol	B02-1964707	1
Fagron	Cholesterol	B02-2015901	1
Fagron	Cholesterol	B02-2015905	1
Fagron	Cholesterol	B02-2022606	6
Fagron	Cholesterol	B20-2135809	1
Fargon / AHD	Cholesterol	16G05-B03-334366	1
Fargon/Alliance	Cholesterol	21C18-B01-213585	2
Fargon/AllianceH.	Cholesterol	16G05-B03-328689	1
Fargon	Cholesterol	19G12-B13-194214	1
Gehe	Cholesterol	B02-2019406	1
Noweda	Cholesterol	15358802	1
Noweda	Cholesterol	15J23-B03-320483	1
Noweda	Cholesterol	17K16-B11-343922	2
Noweda	Cholesterol	19194904	3
Noweda	Cholesterol	22001179013	1
Phönix/Fargon	Cholesterol	17K16-B11-355385	1
Phönix	Cholesterol	19G-12-B13-194214	1
Phönix	Cholesterol	1K16-B11-343922	1
Sanacorp	Cholesterol	21000039010	1
Sanacorp	Cholesterol	22J03-B01-229435	1
Sanacorp	Cholesterol	23003286002	1

- 235 625 spectra from 1515 *Apo-Ident* customers from a total of 49 075 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cholesterol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cholesterol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	220	0	201 864
Type C	0	439	3	235 625

The substance/substance group *Cholesterol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.2727 %)
Type C	100.0000 % (> 99.9007 %)	99.3213 % (> 98.6425 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21219	23760	6.80	125.28
22461	22461	0.00	126.44
22971	22461	21.86	125.39
23760	23760	0.00	123.67
23937	23760	23.00	125.84
25517	22461	8.45	124.43
26160	22461	15.11	125.57
26963	26963	0.00	122.80

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Choline chloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	22639-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Choline chloride; Cholinii chloridum

Special notes

When selecting the *Choline chloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Choline chloride	6	4	0

Second-stage model

For differentiation of the substance/substance group *Choline chloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Choline chloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	111.37	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Choline chloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Choline chloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Choline chloride	162092	22639	40	20160801*
Caelo	Choline chloride	14273819	22663	40	20141002
Caelo	Choline chloride	14273819	22734	40	20141002
Caelo	Choline chloride	16209209	23582	40	20160801
Caelo	Choline chloride	20001839	25557	40	20200721*
Caelo	Choline chloride	21002730	25853	50	20210908*
Fagron	Choline chloride	23C20-B09-230712	26918	40	20230424
Fagron	Choline chloride	23C20-B09-230712	26918SI	20	20230424

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 310 spectra of 8 reference samples from the substance/substance group *Choline chloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 652 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 170 spectra of 5 reference samples from the substance/substance group *Choline chloride*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Choline chloride	172053	23618	40
Caelo	Choline chloride	181082	24264	40
Caelo	Choline chloride	20003488	25662	40
Caelo	Choline chloride	22000199	25990	40
Caelo	Choline chloride	22000199	25990SI	10

- 201 914 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Choline chloride*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Choline chloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Choline chloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	310	0	152 652
Type B	0	170	0	201 914
Type C	0	0	0	236 067

The substance/substance group *Choline chloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0645 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.4706 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22639	22639	0.00	141.53
22663	25853	18.04	140.21
22734	25853	17.41	139.47
23582	22639	10.91	139.43
25557	25557	0.00	151.01
25853	25853	0.00	142.78
26918	25853	10.75	141.34

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Choline hydrogen tartrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20719-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Choline hydrogen tartrate; Cholinium bitartaricum

Special notes

When selecting the *Choline hydrogen tartrate* substance/substance group, the following information is displayed to the user:

- Advice: Currently no longer available from major pharmaceutical manufacturers. Therefore, batch maintenance is currently not possible.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Choline hydrogen tartrate	7	6	5

Second-stage model

For differentiation of the substance/substance group *Choline hydrogen tartrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Choline hydrogen tartrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	150.12	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Choline hydrogen tartrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Choline hydrogen tartrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Choline hydrogen tartrate	1603044	22549	40	20160429*
Euro OTC	Choline hydrogen tartrate	1607020	22689	40	20160808*
Euro OTC	Choline hydrogen tartrate	1603044-01	23010	40	20160429
Euro OTC	Choline hydrogen tartrate	1603044-01	23101	40	20160429
Euro OTC	Choline hydrogen tartrate	1702005	23130	40	20170307*
Euro OTC	Choline hydrogen tartrate	1901053	24484	40	20190228*
Euro OTC	Choline hydrogen tartrate	1910013	24922	40	20191107*
Euro OTC	Choline hydrogen tartrate	2009020	25419	40	20200925*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 320 spectra of 8 reference samples from the substance/substance group *Choline hydrogen tartrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 642 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 260 spectra of 7 reference samples from the substance/substance group *Choline hydrogen tartrate*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Choline hydrogen tartrate	1707023	23610	40
Euro OTC	Choline hydrogen tartrate	1711022	23903	40
Euro OTC	Choline hydrogen tartrate	1802008	23958	40
Euro OTC	Choline hydrogen tartrate	2006031	25303	40
Euro OTC	Choline hydrogen tartrate	2101036	25567	40
Euro OTC	Choline hydrogen tartrate	2110006	25872	50
Euro OTC	Choline hydrogen tartrate	2110006	25872SI	10

- 201 824 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 8 spectra from 4 *Apo-Ident* customers from 6 batches from the substance/substance group *Choline hydrogen tartrate*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Anzag/ Euro OT	Choline hydrogen tartrate	1910013-01	1
Euro OTC	Choline hydrogen tartrate	1309023-01	2
Euro OTC	Choline hydrogen tartrate	1603044-01	1
Euro OTC	Choline hydrogen tartrate	1607020-01	2
Euro OTC	Choline hydrogen tartrate	1707023-01	1
Euro OTC	Choline hydrogen tartrate	1711022-01	1

- 236 059 spectra from 1515 *Apo-Ident* customers from a total of 49 252 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Choline hydrogen tartrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Choline hydrogen tartrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	260	0	201 824
Type C	0	8	0	236 059

The substance/substance group *Choline hydrogen tartrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.6923 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22549	22549	0.00	270.03
22689	22689	0.00	272.54
23010	22549	5.23	272.81
23101	22549	5.27	271.58
23130	23130	0.00	289.84
24484	24484	0.00	278.30
24922	24922	0.00	281.25
25419	25419	0.00	283.77

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ciclopirox olamine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20601-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ciclopirox olamine; Ciclopirox olaminum

Special notes

When selecting the *Ciclopirox olamine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ciclopirox olamine	11	4	96

Second-stage model

For differentiation of the substance/substance group *Ciclopirox olamine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ciclopirox olamine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	83.02	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ciclopirox olamine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ciclopirox olamine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ciclopirox olamine	13343209	21298	40	AR-15-FG-016214-01
Caelo	Ciclopirox olamine	14147406	21655	60	AR-15-FG-014857-01
Caelo	Ciclopirox olamine	14147406	21655SI	60	AR-15-FG-014857-01
Caelo	Ciclopirox olamine	14378809	21991	60	20150227
Caelo	Ciclopirox olamine	14378809	21991SI	60	20150227
Caelo	Ciclopirox olamine	15364408	23011	40	20151201
Caelo	Ciclopirox olamine	15364408	23011SI	40	20151201
Caelo	Ciclopirox olamine	22001499003	26233	40	20220627
Caelo	Ciclopirox olamine	22001499003	26233SI	40	20220627
Caelo	Ciclopirox olamine	24000678	27327	40	20240506*
Caelo	Ciclopirox olamine	24000678	27327SI	40	20240506*
Fagron	Ciclopirox olamine	13A16-N04	21218	40	20130117
Fagron	Ciclopirox olamine	14F13-B03-302340	21964	60	1608170
Fagron	Ciclopirox olamine	14F13-B03-302340	21964SI	60	1608170
Fagron	Ciclopirox olamine	16G26-B02-324884	22969	40	20160907
Fagron	Ciclopirox olamine	16G26-B02-324884	23108	40	20160907
Fagron	Ciclopirox olamine	20B24-F02-370988	25481	40	2102412
Fagron	Ciclopirox olamine	20B24-F02-370988	25481SI	40	2102412
Fagron	Ciclopirox olamine	21B03-B08-210563	25839	50	20210331
Fagron	Ciclopirox olamine	21B03-B08-210563	25839SI	70	20210331

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 960 spectra of 20 reference samples from the substance/substance group *Ciclopirox olamine*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 002 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 400 spectra of 9 reference samples from the substance/substance group *Ciclopirox olamine*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ciclopirox olamine	182102	24280	40
Caelo	Ciclopirox olamine	22003201	26507	40
Fagron	Ciclopirox olamine	14E21-M04	21594	60
Fagron	Ciclopirox olamine	22A11-B03-215669	26176	40
Caelo	Ciclopirox olamine	22003201	26507SI	40
Fagron	Ciclopirox olamine	14E21-M04	21594SI	60
Fagron	Ciclopirox olamine	16G26-B02-324884	22969SI†	40
Fagron	Ciclopirox olamine	16G26-B02-324884	23108SI†	40
Fagron	Ciclopirox olamine	22A11-B03-215669	26176SI	40

- 201 684 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 404 spectra from 171 *Apo-Ident* customers from 102 batches from the substance/substance group *Ciclopirox olamine*.
- Among them are spectra of independent samples from 96 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ciclopirox olamine	22001499004	1
	Ciclopirox olamine	22003201002	1
	Ciclopirox olamine	22003201004	5
	Ciclopirox olamine	22003201009	3
	Ciclopirox olamine	23000858003	1
Cael	Ciclopirox olamine	12040911	2
Caelo	Ciclopirox olamine	12040906	1
Caelo	Ciclopirox olamine	12040911	1
Caelo	Ciclopirox olamine	12B22-N03	1
Caelo	Ciclopirox olamine	13343	1
Caelo	Ciclopirox olamine	13343201	1
Caelo	Ciclopirox olamine	13343203	1
Caelo	Ciclopirox olamine	13343208	2
Caelo	Ciclopirox olamine	13343209	3
Caelo	Ciclopirox olamine	14147402	4
Caelo	Ciclopirox olamine	14147405	1
Caelo	Ciclopirox olamine	14275801	2
Caelo	Ciclopirox olamine	14275802	2
Caelo	Ciclopirox olamine	14378801	2
Caelo	Ciclopirox olamine	14378802	1
Caelo	Ciclopirox olamine	14378803	1
Caelo	Ciclopirox olamine	14378804	2
Caelo	Ciclopirox olamine	14378805	4
Caelo	Ciclopirox olamine	14378806	5
Caelo	Ciclopirox olamine	14378809	3
Caelo	Ciclopirox olamine	14378810	9
Caelo	Ciclopirox olamine	15018802	3
Caelo	Ciclopirox olamine	15018803	2
Caelo	Ciclopirox olamine	15304407	1
Caelo	Ciclopirox olamine	15364402	6
Caelo	Ciclopirox olamine	15364404	2
Caelo	Ciclopirox olamine	15364405	5
Caelo	Ciclopirox olamine	15364407	6
Caelo	Ciclopirox olamine	15364408	4
Caelo	Ciclopirox olamine	15364409	2
Caelo	Ciclopirox olamine	15364412	5
Caelo	Ciclopirox olamine	15364414	1
Caelo	Ciclopirox olamine	15364416	2
Caelo	Ciclopirox olamine	16G26-B02-330862	1
Caelo	Ciclopirox olamine	16G26-B02-337355	3
Caelo	Ciclopirox olamine	17118801	5
Caelo	Ciclopirox olamine	17118802	3
Caelo	Ciclopirox olamine	17118806	11
Caelo	Ciclopirox olamine	17118807	4
Caelo	Ciclopirox olamine	17118808	7
Caelo	Ciclopirox olamine	17118811	4
Caelo	Ciclopirox olamine	17307402	10
Caelo	Ciclopirox olamine	17307403	4
Caelo	Ciclopirox olamine	17307405	6
Caelo	Ciclopirox olamine	173074055727	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ciclopirox olamine	17307408	2
Caelo	Ciclopirox olamine	17307410	8
Caelo	Ciclopirox olamine	1810201	1
Caelo	Ciclopirox olamine	182102002	30
Caelo	Ciclopirox olamine	182102003	6
Caelo	Ciclopirox olamine	182102004	3
Caelo	Ciclopirox olamine	182102007	1
Caelo	Ciclopirox olamine	18210201	17
Caelo	Ciclopirox olamine	18210202	4
Caelo	Ciclopirox olamine	18210203	1
Caelo	Ciclopirox olamine	18210204	1
Caelo	Ciclopirox olamine	18210205	2
Caelo	Ciclopirox olamine	18210209	5
Caelo	Ciclopirox olamine	18210210	14
Caelo	Ciclopirox olamine	18212003	1
Caelo	Ciclopirox olamine	1850000758	1
Caelo	Ciclopirox olamine	21000032002	3
Caelo	Ciclopirox olamine	21000032003	3
Caelo	Ciclopirox olamine	21000032007	2
Caelo	Ciclopirox olamine	21000032008	2
Caelo	Ciclopirox olamine	21000032010	5
Caelo	Ciclopirox olamine	21000032012	1
Caelo	Ciclopirox olamine	21000032015	2
Caelo	Ciclopirox olamine	21000032016	1
Caelo	Ciclopirox olamine	2100032010	1
Caelo	Ciclopirox olamine	21B03-B08-210563	1
Caelo	Ciclopirox olamine	22001499003	5
Caelo	Ciclopirox olamine	22001499004	4
Caelo	Ciclopirox olamine	22001499009	2
Caelo	Ciclopirox olamine	22001499011	2
Caelo	Ciclopirox olamine	22003201002	2
Caelo	Ciclopirox olamine	22003201004	2
Caelo	Ciclopirox olamine	3200003	1
Caesar & Lorenz GmbH	Ciclopirox olamine	171188007	1
Caesar & Loretz GmbH...	Ciclopirox olamine	18210205	1
Caesar & Loretz GmbH...	Ciclopirox olamine	21000032007	1
Caesar & Loretz GmbH/GEHE	Ciclopirox olamine	182102002	1
Caesar & Loretz GmbH/GEHE	Ciclopirox olamine	21000032007	4
Caesar & Loretz GmbH/Gehe	Ciclopirox olamine	22001499004	2
Caesar & Loretz GmbH...	Ciclopirox olamine	21000032008	1
Caesar & Loretz GmbH	Ciclopirox olamine	17307405	1
Caesar & Loretz GmbH	Ciclopirox olamine	17307407	1
Caesar & Loretz GmbH	Ciclopirox olamine	17307410	1
Caesar & Loretz GmbH	Ciclopirox olamine	182102002	6
Caesar & Loretz GmbH	Ciclopirox olamine	182102003	4
Caesar & Loretz GmbH	Ciclopirox olamine	18210201	4
Caesar & Loretz GmbH	Ciclopirox olamine	18210205	1
Caesar & Loretz GmbH	Ciclopirox olamine	18210210	5
Caesar & Loretz GmbH	Ciclopirox olamine	21000032002	4
Caesar & Loretz GmbH	Ciclopirox olamine	21000032003	2
Caesar & Loretz GmbH	Ciclopirox olamine	21000032007	1
Caesar & Loretz GmbH	Ciclopirox olamine	21000032008	2
Caesar & Loretz GmbH	Ciclopirox olamine	21000032010	7
Caesar & Loretz GmbH	Ciclopirox olamine	21000032012	1
Caesar & Loretz GmbH	Ciclopirox olamine	21000032016	2
Caesar & Loretz GmbH	Ciclopirox olamine	22001499004	1
Caesar & Loretz GmbH	Ciclopirox olamine	22001499011	1
Caesar & Loretz GmbH	Ciclopirox olamine	22003201002	1
Caesar & Loretz GmbH	Ciclopirox olamine	22003201004	1
Caesar & Loretz Hild...	Ciclopirox olamine	18210205	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz Hilden	Ciclopirox olamine	17307408	1
Caesar & Loretz Hilden	Ciclopirox olamine	182102002	1
Caesar & Loretz Hilden	Ciclopirox olamine	182102003	1
Cealo	Ciclopirox olamine	14147403	2
Euro OTC	Ciclopirox olamine	14378811	2
Euro OTC	Ciclopirox olamine	17118806	1
Euro OTC	Ciclopirox olamine	1718806	1
Fagron	Ciclopirox olamine	10L09-N03	1
Fagron	Ciclopirox olamine	11h03-n02	1
Fagron	Ciclopirox olamine	12G12-N09	2
Fagron	Ciclopirox olamine	13A16-N04	1
Fagron	Ciclopirox olamine	14378806	1
Fagron	Ciclopirox olamine	14E21-M05	1
Fagron	Ciclopirox olamine	14F13-B03	1
Fagron	Ciclopirox olamine	14F13-B03-302339	1
Fagron	Ciclopirox olamine	16G26-B02	1
Fagron	Ciclopirox olamine	16G26-B02-335198	1
Fagron	Ciclopirox olamine	16G26-B02-348603	1
Fagron	Ciclopirox olamine	19A21-B02-362290	2
Fagron	Ciclopirox olamine	20B24_F02_368880	1
Fagron	Ciclopirox olamine	20B24-F02-372655	1
Fagron	Ciclopirox olamine	21B03B08210563	1
Fagron	Ciclopirox olamine	A160013	1
Fargon/Phönix	Ciclopirox olamine	21B03B08210563	1
Gehe	Ciclopirox olamine	14E21-M04	1
Gehe	Ciclopirox olamine	14F13-B03-302339	1
GEHE	Ciclopirox olamine	15364405	1
Gehe	Ciclopirox olamine	17118808	1
Noweda	Ciclopirox olamine	12040911	1
Noweda	Ciclopirox olamine	12B22-N03	1
Noweda	Ciclopirox olamine	17307404	1
Noweda	Ciclopirox olamine	182102003	1
Noweda	Ciclopirox olamine	18210204	1
Noweda	Ciclopirox olamine	22001499011	1
Pharmachem	Ciclopirox olamine	17118808	1
Phoenix	Ciclopirox olamine	15364412	1
Phönix	Ciclopirox olamine	13A16-N04	1
Phönix	Ciclopirox olamine	17307410	1
Phönix	Ciclopirox olamine	18210209	1
Phönix	Ciclopirox olamine	18210210	2
phönix	Ciclopirox olamine	21000032016	1
Phönix	Ciclopirox olamine	22003201004	1
phönix	Ciclopirox olamine	22003201009	1
Phönix	Ciclopirox olamine	23000858003	2
Sanacorp	Ciclopirox olamine	17118806	1
Sanacorp	Ciclopirox olamine	19A21-B02-362290	1

- 235 663 spectra from 1515 *Apo-Ident* customers from a total of 49 156 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ciclopirox olamine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ciclopirox olamine* and it was

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	960	0	152 002
Type B	0	400	0	201 684
Type C	0	399	5	235 663

The substance/substance group *Ciclopirox olamine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.3750 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.5000 %)
Type C	100.0000 % (> 99.9007 %)	98.7624 % (> 98.0198 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21218	21964	6.87	186.17
21298	21298	0.00	162.72
21655	21655	0.00	170.54
21964	21964	0.00	189.38
21991	21298	7.93	163.37
22969	21964	7.53	183.95
23011	21298	6.81	155.87
23108	21964	6.72	185.22
25481	25481	0.00	145.01
25839	27327	44.69	166.42
26233	21964	23.31	180.47
27327	27327	0.00	165.11

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ciclosporin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20941-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ciclosporin; Ciclosporinum

Special notes

When selecting the *Ciclosporin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ciclosporin	7	8	123

Second-stage model

For differentiation of the substance/substance group *Ciclosporin* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ciclosporin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prednisolon dihydrogen phosphate di…	98.78	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ciclosporin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ciclosporin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ciclosporin	13148604	21474	60	1412541
Caelo	Ciclosporin	13148604	21475	60	20130613
Caelo	Ciclosporin	173327	24401	35	20180111*
Caelo	Ciclosporin	192538	25200	40	20191107*
Euro OTC	Ciclosporin	2002031	25356	40	20200825*
Fagron	Ciclosporin	13D26-N07	20941	40	1402057
Fagron	Ciclosporin	13D26-N07	21671	42	1508429
Fagron	Ciclosporin	18G30_B04-354759	24441	40	20181115
Fagron	Ciclosporin	20B13-F03-368652	25182	40	20200313

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 397 spectra of 9 reference samples from the substance/substance group *Ciclosporin*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 565 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 383 spectra of 13 reference samples from the substance/substance group *Ciclosporin*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ciclosporin	12317707	21082	30
Caelo	Ciclosporin	15278907	22966	40
Caelo	Ciclosporin	171583	23669	40
Euro OTC	Ciclosporin	2209015	26342	40
Euro OTC	Ciclosporin	2304018	26772	40
Euro OTC	Ciclosporin	2405004	27363	40
Fagron	Ciclosporin	16C09-B02-325955	23521	30
Fagron	Ciclosporin	23C01-B04-228703	26667	40
Caelo	Ciclosporin	173327	24401†	5
Euro OTC	Ciclosporin	2209015	26342SI	20
Euro OTC	Ciclosporin	2304018	26772SI	20
Fagron	Ciclosporin	13D26-N07	21671†	18
Fagron	Ciclosporin	23C01-B04-228703	26667SI	20

- 201 701 spectra from a total of 4035 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 440 spectra from 168 *Apo-Ident* customers from 130 batches from the substance/substance group *Ciclosporin*.

- Among them are spectra of independent samples from 123 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ciclosporin	22003878002	14
	Ciclosporin	2203878002	1
	Ciclosporin	23001155005	1
	Ciclosporin	23C01-B04-226120	1
	Ciclosporin	23C01-B04-228702	1
	Ciclosporin	23c01-b04-228703	1
Audor Pharma	Ciclosporin	AP170802HBC	2
Caelo	Ciclosporin	1(192538002)	1
Caelo	Ciclosporin	12165602	3
Caelo	Ciclosporin	12165603	2
Caelo	Ciclosporin	12317702	2
Caelo	Ciclosporin	12317703	1
Caelo	Ciclosporin	12317707	4
Caelo	Ciclosporin	13031303	1
Caelo	Ciclosporin	13031801	1
Caelo	Ciclosporin	13148604	2
Caelo	Ciclosporin	13148606	6
Caelo	Ciclosporin	13346803	3
Caelo	Ciclosporin	13346808	1
Caelo	Ciclosporin	13A28-N04	4
Caelo	Ciclosporin	13D26-N07	4
Caelo	Ciclosporin	14199104	3
Caelo	Ciclosporin	14A15-No1	1
Caelo	Ciclosporin	15049703	4
Caelo	Ciclosporin	15278901	4
Caelo	Ciclosporin	15278902	2
Caelo	Ciclosporin	15278903	3
Caelo	Ciclosporin	15278904	7
Caelo	Ciclosporin	15278910	1
Caelo	Ciclosporin	15278913	1
Caelo	Ciclosporin	15278916	1
Caelo	Ciclosporin	15D23-B05-308853	1
Caelo	Ciclosporin	17158303	7
Caelo	Ciclosporin	17158306	4
Caelo	Ciclosporin	17158309	5
Caelo	Ciclosporin	17332702	6
Caelo	Ciclosporin	17332703	3
Caelo	Ciclosporin	1733702	1
Caelo	Ciclosporin	18041817	1
Caelo	Ciclosporin	18136101	8
Caelo	Ciclosporin	18136104	14
Caelo	Ciclosporin	18136108	5
Caelo	Ciclosporin	19011301	1
Caelo	Ciclosporin	19055803	1
Caelo	Ciclosporin	19055804	18
Caelo	Ciclosporin	19055805	14
Caelo	Ciclosporin	19055807	1
Caelo	Ciclosporin	19055808	2
Caelo	Ciclosporin	19055809	1
Caelo	Ciclosporin	19055810	1
Caelo	Ciclosporin	192538002	9
Caelo	Ciclosporin	192538004	1
Caelo	Ciclosporin	192538005	4
Caelo	Ciclosporin	192538007	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ciclosporin	20E08-F06-371274	1
Caelo	Ciclosporin	21000144001	1
Caelo	Ciclosporin	21000144002	12
Caelo	Ciclosporin	21000144010	6
Caelo	Ciclosporin	21000144012	4
Caelo	Ciclosporin	21000144013	1
Caelo	Ciclosporin	2100144012	1
Caelo	Ciclosporin	21A25-F02-376839	1
Caelo	Ciclosporin	29689114C22B02	1
Caesar & Loretz GmbH...	Ciclosporin	19055805	1
Caesar & Loretz GmbH...	Ciclosporin	21000144010	2
Caesar & Loretz GmbH...	Ciclosporin	192538002	1
Caesar & Loretz GmbH...	Ciclosporin	192538002	1
Caesar & Loretz GmbH...	Ciclosporin	21000144002	1
Caesar & Loretz GmbH	Ciclosporin	17332702	1
Caesar & Loretz GmbH	Ciclosporin	18136104	6
Caesar & Loretz GmbH	Ciclosporin	19055804	1
Caesar & Loretz GmbH	Ciclosporin	19055805	8
Caesar & Loretz GmbH	Ciclosporin	192538002	10
Caesar & Loretz GmbH	Ciclosporin	192538007	6
Caesar & Loretz GmbH	Ciclosporin	21000144002	5
Caesar & Loretz GmbH	Ciclosporin	21000144004	1
Caesar & Loretz GmbH	Ciclosporin	21000144010	7
Caesar & Loretz GmbH	Ciclosporin	21000144011	1
Caesar & Loretz GmbH	Ciclosporin	21000144012	4
Caesar & Loretz GmbH	Ciclosporin	21000941001	1
Caesar & Loretz GmbH	Ciclosporin	F06-3712702	1
Caesar & Loretz	Ciclosporin	17158306	1
Concord Biotech Ltd....	Ciclosporin	14G22-B02-296891	1
Euro OTC	Ciclosporin	256866	1
Fagron	Ciclosporin	10J18-N06	1
Fagron	Ciclosporin	1103531	1
Fagron	Ciclosporin	11K17-N13	1
Fagron	Ciclosporin	12E31-N02	7
Fagron	Ciclosporin	13414038	1
Fagron	Ciclosporin	13417083	2
Fagron	Ciclosporin	13420003	1
Fagron	Ciclosporin	13420023	4
Fagron	Ciclosporin	13420107	1
Fagron	Ciclosporin	13421135	1
Fagron	Ciclosporin	13A28-n04	1
Fagron	Ciclosporin	13A28-N04	4
Fagron	Ciclosporin	13B19N02	2
Fagron	Ciclosporin	13B19-N02	4
Fagron	Ciclosporin	13d026N07	1
Fagron	Ciclosporin	13D26-N07	10
Fagron	Ciclosporin	13H19_N09	1
Fagron	Ciclosporin	13H19-N09	4
Fagron	Ciclosporin	14/18-B02-300180	1
Fagron	Ciclosporin	14718-b02-300180	1
Fagron	Ciclosporin	14a15-n01	1
Fagron	Ciclosporin	14A15-N01	3
Fagron	Ciclosporin	14g22-b02-296891	1
Fagron	Ciclosporin	14G22-B02-296891	5
Fagron	Ciclosporin	15D23-B05	2
Fagron	Ciclosporin	15D23-B05-307217	1
Fagron	Ciclosporin	15D23-B05-308853	7
Fagron	Ciclosporin	15F29-B14	1
Fagron	Ciclosporin	15f29-b14-316270	2
Fagron	Ciclosporin	15F29B14316270	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Ciclosporin	15F29-B14-316270	1
Fagron	Ciclosporin	15F29-B14-321791	1
Fagron	Ciclosporin	15f29-b14-325654	1
Fagron	Ciclosporin	16121401	1
Fagron	Ciclosporin	18136104	1
Fagron	Ciclosporin	18A18-B07-344620	3
Fagron	Ciclosporin	18A18-B07-344621	1
Fagron	Ciclosporin	18A18-B07-344622	1
Fagron	Ciclosporin	18A18-B07-349163	2
Fagron	Ciclosporin	18G30-B04	3
Fagron	Ciclosporin	18G30-B04-0001	1
Fagron	Ciclosporin	18G30-B04-354758	1
Fagron	Ciclosporin	18G30-B04-354759	4
Fagron	Ciclosporin	18G30-B04-3568304	1
Fagron	Ciclosporin	18G30-B04-358809	3
Fagron	Ciclosporin	20B13-F03	2
Fagron	Ciclosporin	20B13-F03-368653	1
Fagron	Ciclosporin	20E08-F06-3124	1
Fagron	Ciclosporin	20E08-F06-371272	2
Fagron	Ciclosporin	20E08-F06-371273	7
Fagron	Ciclosporin	20E08-F06-371275	2
Fagron	Ciclosporin	21A25-F02-376839	2
Fagron	Ciclosporin	21J12-B19-216847	1
Fagron	Ciclosporin	21J12-B19-217253	2
Fagron	Ciclosporin	21K15-B05-215789	3
Fagron	Ciclosporin	21K15-B05-216970	2
Fagron	Ciclosporin	21K15-B05-217761	1
Fagron	Ciclosporin	21L14-B02-219484	2
Fagron	Ciclosporin	21L14-B02-221862	2
Fagron	Ciclosporin	23C01-B04-223807	1
Fagron	Ciclosporin	23C01-B04-226120	2
Fagron	Ciclosporin	25051302	1
Fagron	Ciclosporin	59865-13-3	1
Fargon/Gehe	Ciclosporin	18A18-B07-344620	1
Fargon	Ciclosporin	13D26-No7	1
Gehe	Ciclosporin	17158303	1
Gehe	Ciclosporin	17158306	1
Gehe	Ciclosporin	17332702	1
Gehe	Ciclosporin	17332703	1
Gehe	Ciclosporin	18136101	1
Gehe	Ciclosporin	18136104	1
Gehe	Ciclosporin	22003878002	2
Gehe	Ciclosporin	23001155005	1
Medisca/Ortscheidt	Ciclosporin		1
Noweda	Ciclosporin	23C01-B04-231019	1
Ortscheid 21.10.2021	Ciclosporin		1
Phoenix	Ciclosporin	17158303	1
Phoenix	Ciclosporin	20B13-F03-368653	1
Phönix	Ciclosporin	13D26-N07	1
Sanacorp	Ciclosporin	21000144002	2
Sanacorp	Ciclosporin	23C01-B04-226120	1
VDL	Ciclosporin	13D26-N07	1

- 235 627 spectra from 1515 *Apo-Ident* customers from a total of 49 131 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Ciclosporin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ciclosporin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	397	0	152 565
Type B	0	383	0	201 701
Type C	0	438	2	235 627

The substance/substance group *Ciclosporin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4887 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.4334 %)
Type C	100.0000 % (> 99.9007 %)	99.5455 % (> 98.8636 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20941	20941	0.00	119.69
21474	21474	0.00	129.12
21475	21474	2.89	129.00
21671	21671	0.00	121.50
24401	24401	0.00	128.60
24441	21474	16.07	127.95
25182	20941	13.17	122.19
25200	25200	0.00	127.35
25356	25356	0.00	114.42

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ciprofloxacin hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20945-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ciprofloxacin hydrochloride; Ciprofloxacini hydrochloridum

Special notes

When selecting the *Ciprofloxacin hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ciprofloxacin hydrochloride	6	3	14

Second-stage model

For differentiation of the substance/substance group *Ciprofloxacin hydrochloride* the following second-stage model is used:

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ciprofloxacin hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	121.98	–
⋮	⋮	⋮
Quinine hydrochloride dihydrate	>50	145.02
Sodium citrate	>50	218.52
Methoxsalen	>50	239.32
Capsaicin	>50	301.93
Pyridoxal-5-phosphate	>50	321.92
Oxybutynin hydrochloride	>50	348.87
Prednicarbate	>50	384.07
Levocarnitine	>50	389.52
Heparin sodium	>50	409.69
Cyproterone acetate	>50	473.69
Tetracaine	>50	673.99
Triclosan	>50	763.24
Amitriptyline hydrochloride	>50	960.51
Alfatradiol	>50	1055.06
Norethisterone acetate	>50	1193.48
Valine	>50	1303.32
Sucrose	>50	1402.14
Amifampridine	>50	1844.66

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ciprofloxacin hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ciprofloxacin hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ciprofloxacin hydrochloride	12B08-N03	20945	40	1401421
Fagron	Ciprofloxacin hydrochloride	14B25-B02	21254	40	20140324

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ciprofloxacin hydrochloride	16B17-B05-341882	23938	40	20160302
Fagron	Ciprofloxacin hydrochloride	18F27-B01-353346	24581	40	20180814
Fagron	Ciprofloxacin hydrochloride	20G01-F04-373719	25719	50	20200924
Fagron	Ciprofloxacin hydrochloride	21J08-B07-215636	26330	40	20220315
Fagron	Ciprofloxacin hydrochloride	21J08-B07-215636	26330SI	20	20220315

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 270 spectra of 7 reference samples from the substance/substance group *Ciprofloxacin hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 692 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 5 reference samples from the substance/substance group *Ciprofloxacin hydrochloride*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ciprofloxacin hydrochloride	15D07-B01-312864	22755	40
Fagron	Ciprofloxacin hydrochloride	17K09-B02-345976	23991	40
Fagron	Ciprofloxacin hydrochloride	23F23-B08-228691	26898	40
Fagron	Ciprofloxacin hydrochloride	15D07-B01-312864	23568	40
Fagron	Ciprofloxacin hydrochloride	23F23-B08-228691	26898SI	20

- 201 904 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples

are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 15 spectra from 12 *Apo-Ident* customers from 14 batches from the substance/substance group *Ciprofloxacin hydrochloride*.
- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ciprofloxacin hydrochloride	21J08-B07-223799	1
Caelo	Ciprofloxacin hydrochloride	16B17-B05-324218	1
Fagron	Ciprofloxacin hydrochloride	14/15-B08-303363	1
Fagron	Ciprofloxacin hydrochloride	14B25-B02-291783	2
Fagron	Ciprofloxacin hydrochloride	14B25-B02-291-783	1
Fagron	Ciprofloxacin hydrochloride	14F13-B01-303362	1
Fagron	Ciprofloxacin hydrochloride	14I15-B08	1
Fagron	Ciprofloxacin hydrochloride	14I15-B08-303363	1
Fagron	Ciprofloxacin hydrochloride	14l15-B08	1
Fagron	Ciprofloxacin hydrochloride	15D07-B01-312864	1
Fagron	Ciprofloxacin hydrochloride	17K09-B02-345976	1
Fagron	Ciprofloxacin hydrochloride	18F27-B01-363555	1
Fagron	Ciprofloxacin hydrochloride	CI0A003	1
Fargon/Anzag	Ciprofloxacin hydrochloride	F04-3737109	1

- 236 052 spectra from 1515 *Apo-Ident* customers from a total of 49 244 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ciprofloxacin hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ciprofloxacin hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	270	0	152 692
Type B	0	180	0	201 904
Type C	0	15	0	236 052

The substance/substance group *Ciprofloxacin hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7778 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20945	20945	0.00	207.90
21254	20945	13.37	203.71
23938	20945	36.33	195.61
24581	20945	21.20	200.34
25719	20945	32.29	197.99
26330	20945	25.66	200.68

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Citric acid**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20019-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Citric acid; Acidum citricum

Special notes

When selecting the *Citric acid* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Citric acid	8	25	647

Second-stage model

For differentiation of the substance/substance group *Citric acid* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Citric acid* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Magnesium hydrogen citrate	92.94	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Citric acid* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Citric acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Citric acid	11380204	20682	40	20120127
Caelo	Citric acid	12043112	20683	40	20120229
Caelo	Citric acid	13396502	21455	60	20140110
Caelo	Citric acid	13243213	21487	40	20130821
Caelo	Citric acid	160386	22463	60	20160315*
Caelo	Citric acid	22002250	26350	40	20220912*
Caelo	Citric acid	22002250	26350SI	20	20220912*
Fagron	Citric acid	12F18-N03	20706	40	20120628
Fagron	Citric acid	13G24-N13	20913	40	20130827

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 380 spectra of 9 reference samples from the substance/substance group *Citric acid*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 582 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1170 spectra of 31 reference samples from the substance/substance group *Citric acid*.

- Among them are spectra of independent samples from 25 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Citric acid	160387	22478	60
Caelo	Citric acid	162086	22620	40
Caelo	Citric acid	162154	22622	40
Caelo	Citric acid	171627	23303	40
Caelo	Citric acid	171626	23421	40
Caelo	Citric acid	180976	24034	40
Caelo	Citric acid	181292	24232	40
Caelo	Citric acid	183121	24366	40
Caelo	Citric acid	183071	24367	40
Caelo	Citric acid	192036	24740	40
Caelo	Citric acid	192073	24744	40
Caelo	Citric acid	21000543	25631	40
Caelo	Citric acid	21000544	25635	40
Caelo	Citric acid	21002657	25855	50
Caelo	Citric acid	22000645	26122	40
Caelo	Citric acid	22002309	26358	40
Caelo	Citric acid	23002104	26946	40
Caelo	Citric acid	23002107	26955	40
Caelo	Citric acid	24001159	27253	40
Euro OTC	Citric acid	2112002	25947	40
Euro OTC	Citric acid	2301021	26510	40
Euro OTC	Citric acid	2310005	27007	40
Euro OTC	Citric acid	2407008	27457	40
Fagron	Citric acid	21F11-B04-213849	26146	40
Fagron	Citric acid	23C01-B01-228324	26828	30
Caelo	Citric acid	171626	23648	40
Caelo	Citric acid	171627	23677	40
Caelo	Citric acid	22000645	26122SI	20
Caelo	Citric acid	22002309	26358SI	20

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Citric acid	2112002	25947SI	10
Fagron	Citric acid	21F11-B04-213849	26146SI	20

- 200 914 spectra from a total of 4020 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4343 spectra from 1217 *Apo-Ident* customers from 666 batches from the substance/substance group *Citric acid*.
- Among them are spectra of independent samples from 642 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Citric acid	12345	1
	Citric acid	13K18-B34-291523	1
	Citric acid	2000645001	1
	Citric acid	21000543008	1
	Citric acid	21000543010	1
	Citric acid	21000544002	1
	Citric acid	21002657002	2
	Citric acid	21002657003	1
	Citric acid	21002657006	1
	Citric acid	21002657007	1
	Citric acid	21002657012	4
	Citric acid	21002657015	13
	Citric acid	21002657016	1
	Citric acid	21002657017	7
	Citric acid	2112002-03	2
	Citric acid	220000645004	1
	Citric acid	22000645001	2
	Citric acid	22000645005	1
	Citric acid	22000645009	6
	Citric acid	22000645011	5
	Citric acid	220021564	1
	Citric acid	22002250001	5
	Citric acid	22002250004	2
	Citric acid	22002309001	7
	Citric acid	22002309004	10
	Citric acid	22H11-B02-227794	1
	Citric acid	22I05-B07-222923	1
	Citric acid	22I05-B07-225242	1
	Citric acid	23003597001	1
	Citric acid	2301021-01	1
	Citric acid	23568	1
	Citric acid	6491041	1
092522438	Citric acid	22000645001	2
12.12.2016 Phoenix 4,59EUR	Citric acid	15088008	1
A.H. 08.06.13 ek: 6,92EUR	Citric acid	13050604	1
AEP	Citric acid	22002309004	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
AHD	Citric acid	13050607	1
AHD	Citric acid	13396502	1
AHD	Citric acid	15063218	1
AHD	Citric acid	16208614	1
AHD	Citric acid	17329511	2
AHD	Citric acid	20000886003	1
AHD	Citric acid	21000543008	1
AHD	Citric acid	21002657003	1
AHD	Citric acid	21002657015	2
AHD	Citric acid	22000645001	1
ALH	Citric acid	L1508013-01	1
Alliance Health 03.0...	Citric acid	13K18-B34	1
Alliance Healthcare	Citric acid	12043123	1
ALLIANCE HEALTHCARE	Citric acid	19003185	1
Alliance Healthcare	Citric acid	21000543008	1
Anzag	Citric acid	10049712	1
Anzag	Citric acid	10049713	1
anzag	Citric acid	13175409	1
Anzag	Citric acid	192073009	2
Anzag	Citric acid	21002657017	1
Anzag	Citric acid	6494061	1
apomix	Citric acid	16208612	2
Apotheke	Citric acid	21000543005	1
Audor Pharma	Citric acid	PA201	1
Beyvers	Citric acid	16038606	1
Bombastus	Citric acid	12250004-3-0	1
Bombastus	Citric acid	13396502	1
Bombastus	Citric acid	17162601	2
Bombastus	Citric acid	17162602	1
Bombastus	Citric acid	18097060	1
Bombastus	Citric acid	20002872	1
Bombastus	Citric acid	21004820	1
Bombastus	Citric acid	272757	2
Caelo	Citric acid		10
Caelo	Citric acid	10049716	1
Caelo	Citric acid	1015U-01024	1
Caelo	Citric acid	10182420	1
Caelo	Citric acid	1044905	1
Caelo	Citric acid	1072015B	1
Caelo	Citric acid	11066806	1
Caelo	Citric acid	11159801	2
Caelo	Citric acid	11159817	1
Caelo	Citric acid	11159821	1
Caelo	Citric acid	11159824	1
Caelo	Citric acid	11178303	5
Caelo	Citric acid	11189817	1
Caelo	Citric acid	11380204	5
Caelo	Citric acid	11380208	1
Caelo	Citric acid	11380213	1
Caelo	Citric acid	11380215	3
Caelo	Citric acid	11380217	2
Caelo	Citric acid	1150817/16208614	1
Caelo	Citric acid	1155609	2
Caelo	Citric acid	1172673	1
Caelo	Citric acid	1175409	2
Caelo	Citric acid	1181765	2
Caelo	Citric acid	11C24-N02	1
Caelo	Citric acid	11C24-N03	1
Caelo	Citric acid	11K07-N01	1
Caelo	Citric acid	11K11-N02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citric acid	12043105	2
Caelo	Citric acid	12043110	4
Caelo	Citric acid	12043112	3
Caelo	Citric acid	12043113	3
Caelo	Citric acid	12043118	3
Caelo	Citric acid	12043119	1
Caelo	Citric acid	12043120	5
Caelo	Citric acid	12043123	6
Caelo	Citric acid	12043124	3
Caelo	Citric acid	12156801	2
Caelo	Citric acid	12156803	8
Caelo	Citric acid	12156804	3
Caelo	Citric acid	12156811	11
Caelo	Citric acid	12156812	4
Caelo	Citric acid	12156818	1
Caelo	Citric acid	12156822	2
Caelo	Citric acid	12156823	4
Caelo	Citric acid	12156824	5
Caelo	Citric acid	12156827	1
Caelo	Citric acid	12156830	1
Caelo	Citric acid	12156832	7
Caelo	Citric acid	121568704	1
Caelo	Citric acid	12175708	3
Caelo	Citric acid	12175711	1
Caelo	Citric acid	12175716	2
Caelo	Citric acid	12175717	1
Caelo	Citric acid	12175718	1
Caelo	Citric acid	1218A-01024	2
Caelo	Citric acid	1230616	1
Caelo	Citric acid	12345	1
Caelo	Citric acid	12353613	1
Caelo	Citric acid	125356	1
Caelo	Citric acid	12B01-N01	5
Caelo	Citric acid	13011801	1
Caelo	Citric acid	13031502	1
Caelo	Citric acid	13050601	9
Caelo	Citric acid	13050604	13
Caelo	Citric acid	13050606	2
Caelo	Citric acid	13050607	9
Caelo	Citric acid	13050610	6
Caelo	Citric acid	13050611	6
Caelo	Citric acid	13050613	18
Caelo	Citric acid	13050614	7
Caelo	Citric acid	13050617	12
Caelo	Citric acid	13050618	3
Caelo	Citric acid	13050621	2
Caelo	Citric acid	13050622	7
Caelo	Citric acid	13050623	2
Caelo	Citric acid	13050623-3376319052	1
Caelo	Citric acid	13050624	1
Caelo	Citric acid	1305601	1
Caelo	Citric acid	13061502	1
Caelo	Citric acid	1306911	1
Caelo	Citric acid	130-7612	1
Caelo	Citric acid	13157404	1
Caelo	Citric acid	13175402	3
Caelo	Citric acid	13175403	14
Caelo	Citric acid	13175404	4
Caelo	Citric acid	13175405	5
Caelo	Citric acid	13175406	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citric acid	13175409	20
Caelo	Citric acid	13175410	4
Caelo	Citric acid	13175411	10
Caelo	Citric acid	13175414	2
Caelo	Citric acid	13175426	4
Caelo	Citric acid	13243005	1
Caelo	Citric acid	13243201	17
Caelo	Citric acid	13243202	10
Caelo	Citric acid	13243208	2
Caelo	Citric acid	13243210	10
Caelo	Citric acid	13243213	21
Caelo	Citric acid	13243214	15
Caelo	Citric acid	13243216	11
Caelo	Citric acid	13243217	6
Caelo	Citric acid	13243218	9
Caelo	Citric acid	13243219	4
Caelo	Citric acid	13243220	2
Caelo	Citric acid	13243221	8
Caelo	Citric acid	13243222	1
Caelo	Citric acid	13243224	2
Caelo	Citric acid	13243225	4
Caelo	Citric acid	13243229	2
Caelo	Citric acid	133243218	1
Caelo	Citric acid	13396502	3
Caelo	Citric acid	13396504	3
Caelo	Citric acid	13396505	3
Caelo	Citric acid	13396506	1
Caelo	Citric acid	13396515	2
Caelo	Citric acid	1380208	1
Caelo	Citric acid	1396505	1
Caelo	Citric acid	13A04-N04	4
Caelo	Citric acid	13D29-N02	1
Caelo	Citric acid	13G24N13	2
Caelo	Citric acid	13G24-N13	4
Caelo	Citric acid	13K18-B34	1
Caelo	Citric acid	13K18-B34-288371TEST	1
Caelo	Citric acid	13K18-B34-288372	1
Caelo	Citric acid	13K18-B34-291520	1
Caelo	Citric acid	13K18-B34-291522	1
Caelo	Citric acid	13K18-B34-291523	2
Caelo	Citric acid	14041506	1
Caelo	Citric acid	14071501	1
Caelo	Citric acid	14162701	1
Caelo	Citric acid	14186301	23
Caelo	Citric acid	14186302	14
Caelo	Citric acid	14186312	16
Caelo	Citric acid	14186313	11
Caelo	Citric acid	14186314	4
Caelo	Citric acid	1418E-01024	1
Caelo	Citric acid	14E06-B07	1
Caelo	Citric acid	14G04-B09	1
Caelo	Citric acid	14G04-B09-293874	2
Caelo	Citric acid	14G04-B09-293876	4
Caelo	Citric acid	14G04B09293877	1
Caelo	Citric acid	14K05-B04-302815	1
Caelo	Citric acid	1501-B06-324348	1
Caelo	Citric acid	15044901	9
Caelo	Citric acid	15044902	4
Caelo	Citric acid	15044903	5
Caelo	Citric acid	15044904	10

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citric acid	15044905	10
Caelo	Citric acid	15063003	26
Caelo	Citric acid	15063003-20160615Ma1	1
Caelo	Citric acid	15063006	5
Caelo	Citric acid	150632	1
Caelo	Citric acid	15063202	1
Caelo	Citric acid	15063203	15
Caelo	Citric acid	15063204	14
Caelo	Citric acid	15063205	3
Caelo	Citric acid	15063206	23
Caelo	Citric acid	15063211	5
Caelo	Citric acid	15063213	27
Caelo	Citric acid	15063214	9
Caelo	Citric acid	15063217	12
Caelo	Citric acid	15063218	11
Caelo	Citric acid	15087510	1
Caelo	Citric acid	15087902	3
Caelo	Citric acid	15087903	19
Caelo	Citric acid	15087904	1
Caelo	Citric acid	15088008	2
Caelo	Citric acid	15088016	4
Caelo	Citric acid	15088017	2
Caelo	Citric acid	15091401	1
Caelo	Citric acid	15124202	1
Caelo	Citric acid	15124301	10
Caelo	Citric acid	15124303	1
Caelo	Citric acid	1516Q-01024	1
Caelo	Citric acid	15185320	1
Caelo	Citric acid	15214301	1
Caelo	Citric acid	15G16-B01-330449	2
Caelo	Citric acid	15G16-B01-330450	1
Caelo	Citric acid	16004701	21
Caelo	Citric acid	16004702	28
Caelo	Citric acid	16004705	4
Caelo	Citric acid	16004706	23
Caelo	Citric acid	16038602	3
Caelo	Citric acid	16038603	5
Caelo	Citric acid	16038604	9
Caelo	Citric acid	16038606	24
Caelo	Citric acid	16038607	7
Caelo	Citric acid	16038608	14
Caelo	Citric acid	16038613	10
Caelo	Citric acid	16038614	5
Caelo	Citric acid	16038617	2
Caelo	Citric acid	16038621	19
Caelo	Citric acid	16038622	9
Caelo	Citric acid	16038701	5
Caelo	Citric acid	16038704	12
Caelo	Citric acid	16038707	11
Caelo	Citric acid	16038708	9
Caelo	Citric acid	16038709	6
Caelo	Citric acid	16038710	3
Caelo	Citric acid	16038712	7
Caelo	Citric acid	16038713	1
Caelo	Citric acid	160607AC	1
Caelo	Citric acid	160614	1
Caelo	Citric acid	1606141	1
Caelo	Citric acid	160808/3	1
Caelo	Citric acid	16088607	1
Caelo	Citric acid	1620610	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citric acid	16206813	1
Caelo	Citric acid	16208605	16
Caelo	Citric acid	162086055525	1
Caelo	Citric acid	16208606	31
Caelo	Citric acid	16208607	33
Caelo	Citric acid	16208608	6
Caelo	Citric acid	16208610	14
Caelo	Citric acid	16208612	25
Caelo	Citric acid	16208613	13
Caelo	Citric acid	16208614	56
Caelo	Citric acid	16208615	3
Caelo	Citric acid	162088606	1
Caelo	Citric acid	162154	1
Caelo	Citric acid	16215403	3
Caelo	Citric acid	16215405	6
Caelo	Citric acid	16215408	6
Caelo	Citric acid	16215409	10
Caelo	Citric acid	170607C/16208605	1
Caelo	Citric acid	17071301	1
Caelo	Citric acid	17161601	1
Caelo	Citric acid	17162601	34
Caelo	Citric acid	17162602	29
Caelo	Citric acid	17162603	9
Caelo	Citric acid	17162604	3
Caelo	Citric acid	1716262601	1
Caelo	Citric acid	17162701	32
Caelo	Citric acid	17162702	12
Caelo	Citric acid	17162706	1
Caelo	Citric acid	1716271	1
Caelo	Citric acid	171652601	1
Caelo	Citric acid	173295002	1
Caelo	Citric acid	17329502	20
Caelo	Citric acid	17329503	8
Caelo	Citric acid	17329504	2
Caelo	Citric acid	17329511	10
Caelo	Citric acid	17329512	3
Caelo	Citric acid	17329513	3
Caelo	Citric acid	177162601	1
Caelo	Citric acid	17E15-B04-335435	1
Caelo	Citric acid	17E15-B04-339371	1
Caelo	Citric acid	180257004	1
Caelo	Citric acid	18025701	48
Caelo	Citric acid	18025702	55
Caelo	Citric acid	18025704	22
Caelo	Citric acid	180257045617	1
Caelo	Citric acid	18025801	30
Caelo	Citric acid	18025802	6
Caelo	Citric acid	180297609	1
Caelo	Citric acid	18091409	1
Caelo	Citric acid	18097202	1
Caelo	Citric acid	18097601	48
Caelo	Citric acid	18097602	15
Caelo	Citric acid	18097603	25
Caelo	Citric acid	18097604	1
Caelo	Citric acid	18097606	19
Caelo	Citric acid	18097607	21
Caelo	Citric acid	18097609	33
Caelo	Citric acid	18097610	1
Caelo	Citric acid	18097611	24
Caelo	Citric acid	18097615	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citric acid	18111704	1
Caelo	Citric acid	1812104	1
Caelo	Citric acid	1812905	2
Caelo	Citric acid	18129204	3
Caelo	Citric acid	18129205	37
Caelo	Citric acid	18129206	4
Caelo	Citric acid	18129207	5
Caelo	Citric acid	183006905	1
Caelo	Citric acid	18304909	1
Caelo	Citric acid	18306902	34
Caelo	Citric acid	18306903	27
Caelo	Citric acid	18306905	50
Caelo	Citric acid	18306905P-190531-4	1
Caelo	Citric acid	18306906	50
Caelo	Citric acid	18306908	9
Caelo	Citric acid	18306909	39
Caelo	Citric acid	18306911	65
Caelo	Citric acid	18306913	2
Caelo	Citric acid	183069606	1
Caelo	Citric acid	18306999	1
Caelo	Citric acid	18307101	2
Caelo	Citric acid	18307102	12
Caelo	Citric acid	18307104	17
Caelo	Citric acid	1831209	1
Caelo	Citric acid	18312102	3
Caelo	Citric acid	18312103	2
Caelo	Citric acid	18312104	18
Caelo	Citric acid	18312107	1
Caelo	Citric acid	18312109	10
Caelo	Citric acid	1836911	1
Caelo	Citric acid	18F25-B02	1
Caelo	Citric acid	18F25-B02-351453	1
Caelo	Citric acid	18F25-B02-351454	1
Caelo	Citric acid	19041304	1
Caelo	Citric acid	19041305	1
Caelo	Citric acid	1917A-01024	1
Caelo	Citric acid	192036002	5
Caelo	Citric acid	192036003	27
Caelo	Citric acid	1920366003	1
Caelo	Citric acid	192037005	1
Caelo	Citric acid	192073002	32
Caelo	Citric acid	192073003	18
Caelo	Citric acid	192073003P-200602-1	1
Caelo	Citric acid	192073004	43
Caelo	Citric acid	192073005	33
Caelo	Citric acid	192073005P-200507-3	1
Caelo	Citric acid	192073005P-200609-5	1
Caelo	Citric acid	192073009	27
Caelo	Citric acid	192073010	2
Caelo	Citric acid	19H23-B07-194438	1
Caelo	Citric acid	200000886003	1
Caelo	Citric acid	200003515014	1
Caelo	Citric acid	200008860003	1
Caelo	Citric acid	20000886001	2
Caelo	Citric acid	20000886002	44
Caelo	Citric acid	20000886003	65
Caelo	Citric acid	20000886006	1
Caelo	Citric acid	20000886007	30
Caelo	Citric acid	20000886009	39
Caelo	Citric acid	20000886012	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citric acid	20000889002	1
Caelo	Citric acid	20003515003	16
Caelo	Citric acid	20003515007	1
Caelo	Citric acid	20003515008	4
Caelo	Citric acid	20003515009	1
Caelo	Citric acid	20003515010	4
Caelo	Citric acid	20003515013	1
Caelo	Citric acid	20003515014	8
Caelo	Citric acid	2000886007	2
Caelo	Citric acid	20060912-3	1
Caelo	Citric acid	20151112-1	1
Caelo	Citric acid	2017-04-18AVLu	1
Caelo	Citric acid	20170728/Ma1	1
Caelo	Citric acid	2019Q-01024	1
Caelo	Citric acid	2051703	1
Caelo	Citric acid	2071303	1
Caelo	Citric acid	20F19-B01-201169	1
Caelo	Citric acid	210000200004	1
Caelo	Citric acid	21000020004	2
Caelo	Citric acid	210000543005	1
Caelo	Citric acid	210000543011	1
Caelo	Citric acid	21000211004	1
Caelo	Citric acid	210002657003	1
Caelo	Citric acid	2100054002	1
Caelo	Citric acid	21000542008	1
Caelo	Citric acid	21000543001	1
Caelo	Citric acid	21000543002	8
Caelo	Citric acid	21000543003	20
Caelo	Citric acid	21000543004	1
Caelo	Citric acid	21000543005	13
Caelo	Citric acid	21000543006	3
Caelo	Citric acid	21000543008	21
Caelo	Citric acid	21000543010	5
Caelo	Citric acid	21000543011	6
Caelo	Citric acid	21000544001	11
Caelo	Citric acid	21000544002	58
Caelo	Citric acid	21000544003	2
Caelo	Citric acid	21000544004	10
Caelo	Citric acid	21000544006	8
Caelo	Citric acid	2100054401	1
Caelo	Citric acid	2100054402	1
Caelo	Citric acid	2100054404	1
Caelo	Citric acid	210005543003	1
Caelo	Citric acid	21002657001	9
Caelo	Citric acid	21002657002	10
Caelo	Citric acid	21002657003	32
Caelo	Citric acid	21002657004	1
Caelo	Citric acid	21002657006	9
Caelo	Citric acid	21002657012	5
Caelo	Citric acid	21002657015	12
Caelo	Citric acid	21002657016	4
Caelo	Citric acid	2100543006	1
Caelo	Citric acid	2100544002	1
Caelo	Citric acid	2100544004	1
Caelo	Citric acid	21531	1
Caelo	Citric acid	22000645001	8
Caelo	Citric acid	22000645004	2
Caelo	Citric acid	22000645005	2
Caelo	Citric acid	22000645008	1
Caelo	Citric acid	22002309004	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citric acid	2317M-01024	1
Caelo	Citric acid	2317Q-01024	1
Caelo	Citric acid	24021502	1
Caelo	Citric acid	26051803	1
Caelo	Citric acid	26071701	1
Caelo	Citric acid	26111301	1
Caelo	Citric acid	2617Q-01024	1
Caelo	Citric acid	27091303	1
Caelo	Citric acid	2716A-01024	1
Caelo	Citric acid	2789	1
Caelo	Citric acid	28021405	1
Caelo	Citric acid	28051401	1
Caelo	Citric acid	3091701	1
Caelo	Citric acid	3275	1
Caelo	Citric acid	4918Q-01024	1
Caelo	Citric acid	501170606	1
Caelo	Citric acid	5041802	1
Caelo	Citric acid	5315I-01024	1
Caelo	Citric acid	59(20000886009)	1
Caelo	Citric acid	6071713	1
Caelo	Citric acid	6498011	2
Caelo	Citric acid	713I-01024	1
Caelo	Citric acid	7808	2
Caelo	Citric acid	8031702	1
Caelo	Citric acid	8306911	1
Caelo	Citric acid	886007	1
Caelo	Citric acid	9158408	1
Caelo	Citric acid	9199105	1
Caelo	Citric acid	9494185	1
Caelo	Citric acid	A-040513-1	1
Caelo	Citric acid	AP220721-01	1
Caelo	Citric acid	jjjjjj	1
Caelo	Citric acid	L130404202	1
Caelo	Citric acid	L1508013-01	1
Caelo	Citric acid	L1609021-01	3
Caelo	Citric acid	L1805017-03	2
Caelo	Citric acid	P-12061921/18097611	1
Caelo	Citric acid	P-12081922/18312102	1
Caelo	Citric acid	P170612AC06/19	1
Caelo	Citric acid	xxxx	1
Caelo	Citric acid	xxxxxx	1
Caeolo/Gehe	Citric acid	15044903	3
Caesar & Lorenz GmbH	Citric acid	16004706	1
Caesar & Lorenz	Citric acid	21002657003	1
Caesar & Loretz /Sanacorp	Citric acid	20000886002	1
Caesar & Loretz GmbH...	Citric acid	22002309004	1
Caesar & Loretz GmbH...	Citric acid	16208614	1
Caesar & Loretz GmbH...	Citric acid	15063203	1
Caesar & Loretz GmbH...	Citric acid	192073002	1
Caesar & Loretz GmbH...	Citric acid	21000543003	1
Caesar & Loretz GmbH...	Citric acid	18306906	1
Caesar & Loretz GmbH...	Citric acid	20000886009	1
Caesar & Loretz GmbH...	Citric acid	18025702	1
Caesar & Loretz GmbH...	Citric acid	18097609	2
Caesar & Loretz GmbH...	Citric acid	18097611	1
Caesar & Loretz GmbH...	Citric acid	192073003	1
Caesar & Loretz GmbH...	Citric acid	192073005	1
Caesar & Loretz GmbH...	Citric acid	192073009	1
Caesar & Loretz GmbH...	Citric acid	21000544006	1
Caesar & Loretz GmbH...	Citric acid	21000544001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Citric acid	18306905	1
Caesar & Loretz GmbH...	Citric acid	21000544002	1
Caesar & Loretz GmbH /G	Citric acid	18306911	1
Caesar & Loretz GmbH/ AEP	Citric acid	192073003	1
Caesar & Loretz GmbH...	Citric acid	17162712	1
Caesar & Loretz GmbH...	Citric acid	18306909	1
Caesar & Loretz GmbH...	Citric acid	192073009	1
Caesar & Loretz GmbH...	Citric acid	20000886003	1
Caesar & Loretz GmbH/AEP	Citric acid	192073005	1
Caesar & Loretz GmbH/AEP	Citric acid	21002657001	1
Caesar & Loretz GmbH/AHD	Citric acid	18306906	1
Caesar & Loretz GmbH/AHD	Citric acid	192073005	2
Caesar & Loretz GmbH/AHD	Citric acid	20000886003	1
Caesar & Loretz GmbH/AHD	Citric acid	21000544002	1
Caesar & Loretz GmbH...	Citric acid	21000543011	1
Caesar & Loretz GmbH...	Citric acid	21000544001	1
Caesar & Loretz GmbH...	Citric acid	21000544002	1
Caesar & Loretz GmbH...	Citric acid	20000886003	1
Caesar & Loretz GmbH/E	Citric acid	21000543003	1
Caesar & Loretz GmbH...	Citric acid	18306902	1
Caesar & Loretz GmbH...	Citric acid	192073009	1
Caesar & Loretz GmbH...	Citric acid	21000543010	1
Caesar & Loretz GmbH/Gehe	Citric acid	18129211	1
Caesar & Loretz GmbH/Gehe	Citric acid	18306905	1
Caesar & Loretz GmbH/Gehe	Citric acid	18306911	1
Caesar & Loretz GmbH/Gehe	Citric acid	18307104	1
Caesar & Loretz GmbH/Gehe	Citric acid	18312107	1
Caesar & Loretz GmbH/Gehe	Citric acid	192073005	1
Caesar & Loretz GmbH/Gehe	Citric acid	192073009	2
Caesar & Loretz GmbH/Gehe	Citric acid	20000886007	1
Caesar & Loretz GmbH/Gehe	Citric acid	20000886009	1
Caesar & Loretz GmbH/Gehe	Citric acid	20003515003	1
Caesar & Loretz GmbH/GEHE	Citric acid	20003515004	1
Caesar & Loretz GmbH/GEHE	Citric acid	21000544001	1
Caesar & Loretz GmbH...	Citric acid	21002657006	1
Caesar & Loretz GmbH...	Citric acid	19073004	1
Caesar & Loretz GmbH...	Citric acid	192073009	1
Caesar & Loretz GmbH...	Citric acid	20000886003	1
Caesar & Loretz GmbH...	Citric acid	21000544002	1
Caesar & Loretz GmbH...	Citric acid	22002309004	1
Caesar & Loretz GmbH...	Citric acid	18306909	2
Caesar & Loretz GmbH...	Citric acid	18306911	1
Caesar & Loretz GmbH...	Citric acid	20003515003	1
Caesar & Loretz GmbH...	Citric acid	20000886002	2
Caesar & Loretz GmbH...	Citric acid	21000543005	2
Caesar & Loretz GmbH...	Citric acid	21000543006	4
Caesar & Loretz GmbH...	Citric acid	18306906	2
Caesar & Loretz GmbH...	Citric acid	18306908	1
Caesar & Loretz GmbH...	Citric acid	192073003	4
Caesar & Loretz GmbH...	Citric acid	21000543002	3
Caesar & Loretz GmbH...	Citric acid	21000543008	2
Caesar & Loretz GmbH...	Citric acid	21000544002	2
Caesar & Loretz GmbH...	Citric acid	21002657002	1
Caesar & Loretz GmbH/P	Citric acid	192073002	1
Caesar & Loretz GmbH...	Citric acid	18097611	3
Caesar & Loretz GmbH...	Citric acid	18306905	1
Caesar & Loretz GmbH...	Citric acid	2000886003	1
Caesar & Loretz GmbH...	Citric acid	21000544002	1
Caesar & Loretz GmbH...	Citric acid	21002657002	1
Caesar & Loretz GmbH...	Citric acid	21000543006	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Citric acid	18097606	1
Caesar & Loretz GmbH...	Citric acid	18306906	1
Caesar & Loretz GmbH...	Citric acid	18306908	1
Caesar & Loretz GmbH...	Citric acid	18307104	1
Caesar & Loretz GmbH...	Citric acid	192073002	1
Caesar & Loretz GmbH...	Citric acid	20000886007	1
Caesar & Loretz GmbH...	Citric acid	20000886009	1
Caesar & Loretz GmbH...	Citric acid	21000543008	1
Caesar & Loretz GmbH...	Citric acid	21000544002	1
Caesar & Loretz GmbH...	Citric acid	21002657002	1
Caesar & Loretz GmbH...	Citric acid	21002657015	1
Caesar & Loretz GmbH...	Citric acid	192073002	1
Caesar & Loretz GmbH/Sa	Citric acid	192073003	2
Caesar & Loretz GmbH...	Citric acid	192036004	1
Caesar & Loretz GmbH/Sana	Citric acid	20000886009	1
Caesar & Loretz GmbH...	Citric acid	192036009	1
Caesar & Loretz GmbH...	Citric acid	18306909	1
Caesar & Loretz GmbH...	Citric acid	18312104	2
Caesar & Loretz GmbH...	Citric acid	192073003	1
Caesar & Loretz GmbH...	Citric acid	20003515003	1
Caesar & Loretz GmbH...	Citric acid	21000544002	1
Caesar & Loretz GmbH...	Citric acid	21002657001	1
Caesar & Loretz GmbH/Sani	Citric acid	20003515003	1
Caesar & Loretz GmbH	Citric acid	13243201	1
Caesar & Loretz GmbH	Citric acid	13243214	1
Caesar & Loretz GmbH	Citric acid	15063003	2
Caesar & Loretz GmbH	Citric acid	15063203	1
Caesar & Loretz GmbH	Citric acid	16208607	1
Caesar & Loretz GmbH	Citric acid	16208614	1
Caesar & Loretz GmbH	Citric acid	162154403	1
Caesar & Loretz GmbH	Citric acid	17162602	1
Caesar & Loretz GmbH	Citric acid	17162701	1
Caesar & Loretz GmbH	Citric acid	17329502	1
Caesar & Loretz GmbH	Citric acid	18025701	1
Caesar & Loretz GmbH	Citric acid	18097606	1
Caesar & Loretz GmbH	Citric acid	18097611	2
Caesar & Loretz GmbH	Citric acid	18129204	1
Caesar & Loretz GmbH	Citric acid	18129205	2
Caesar & Loretz GmbH	Citric acid	18129207	1
Caesar & Loretz GmbH	Citric acid	18306902	5
Caesar & Loretz GmbH	Citric acid	18306903	7
Caesar & Loretz GmbH	Citric acid	18306904	2
Caesar & Loretz GmbH	Citric acid	18306905	17
Caesar & Loretz GmbH	Citric acid	18306906	13
Caesar & Loretz GmbH	Citric acid	18306908	3
Caesar & Loretz GmbH	Citric acid	18306909	13
Caesar & Loretz GmbH	Citric acid	18306911	15
Caesar & Loretz GmbH	Citric acid	18307102	2
Caesar & Loretz GmbH	Citric acid	18307104	4
Caesar & Loretz GmbH	Citric acid	18312103	1
Caesar & Loretz GmbH	Citric acid	18312104	9
Caesar & Loretz GmbH	Citric acid	18312107	2
Caesar & Loretz GmbH	Citric acid	18312109	1
Caesar & Loretz GmbH	Citric acid	18F25-B02	1
Caesar & Loretz GmbH	Citric acid	18F25-B02_351454	1
Caesar & Loretz GmbH	Citric acid	192036002	2
Caesar & Loretz GmbH	Citric acid	192036003	18
Caesar & Loretz GmbH	Citric acid	192036004	2
Caesar & Loretz GmbH	Citric acid	192036009	1
Caesar & Loretz GmbH	Citric acid	192073002	10

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Citric acid	192073003	4
Caesar & Loretz GmbH	Citric acid	192073004	8
Caesar & Loretz GmbH	Citric acid	192073005	10
Caesar & Loretz GmbH	Citric acid	192073009	8
Caesar & Loretz GmbH	Citric acid	192073010	4
Caesar & Loretz GmbH	Citric acid	19H23-B07	1
Caesar & Loretz GmbH	Citric acid	200000886003	1
Caesar & Loretz GmbH	Citric acid	20000886002	16
Caesar & Loretz GmbH	Citric acid	20000886003	7
Caesar & Loretz GmbH	Citric acid	20000886007	7
Caesar & Loretz GmbH	Citric acid	20000886008	3
Caesar & Loretz GmbH	Citric acid	20000886009	13
Caesar & Loretz GmbH	Citric acid	20003515002	2
Caesar & Loretz GmbH	Citric acid	20003515003	4
Caesar & Loretz GmbH	Citric acid	20003515004	1
Caesar & Loretz GmbH	Citric acid	20003515008	1
Caesar & Loretz GmbH	Citric acid	20003515010	2
Caesar & Loretz GmbH	Citric acid	20003515014	2
Caesar & Loretz GmbH	Citric acid	21000020004	1
Caesar & Loretz GmbH	Citric acid	210000544002	1
Caesar & Loretz GmbH	Citric acid	21000543002	2
Caesar & Loretz GmbH	Citric acid	21000543003	6
Caesar & Loretz GmbH	Citric acid	21000543005	4
Caesar & Loretz GmbH	Citric acid	21000543008	5
Caesar & Loretz GmbH	Citric acid	21000543010	6
Caesar & Loretz GmbH	Citric acid	21000543011	1
Caesar & Loretz GmbH	Citric acid	21000544001	6
Caesar & Loretz GmbH	Citric acid	21000544002	20
Caesar & Loretz GmbH	Citric acid	21000544004	13
Caesar & Loretz GmbH	Citric acid	21000544006	4
Caesar & Loretz GmbH	Citric acid	21002657001	4
Caesar & Loretz GmbH	Citric acid	21002657002	3
Caesar & Loretz GmbH	Citric acid	21002657003	11
Caesar & Loretz GmbH	Citric acid	21002657006	3
Caesar & Loretz GmbH	Citric acid	21002657015	3
Caesar & Loretz GmbH	Citric acid	21002657016	1
Caesar & Loretz GmbH	Citric acid	2100543003	1
Caesar & Loretz GmbH	Citric acid	22000645001	3
Caesar & Loretz Hilden	Citric acid	18312104	1
Caesar & Loretz Hilden	Citric acid	18312109	1
Caesar & Loretz/ Noweda	Citric acid	12156812	1
Caesar & Loretz/Geil...	Citric acid	20003515003	1
Caesar & Loretz/Noweda	Citric acid	20003515003	1
Caesar & Loretz	Citric acid	15087904	2
Caesar & Loretz	Citric acid	16038613	1
Caesar & Loretz	Citric acid	18097603	1
Caesar & Loretz	Citric acid	18307102	1
Caesar / Gehe	Citric acid	15087904	1
Caesar u. Loretz GmbH	Citric acid	18307104	1
Caesar u. Loretz GmbH	Citric acid	192073005	1
Caesar u. Loretz GmbH	Citric acid	21000544001	1
Caesar und Loretz	Citric acid	18306911	1
Caesar&Lorenz	Citric acid	21000544002	1
Caesar&Loretz GmbH,1...	Citric acid	16004706	1
Caesar&Loretz GmbH	Citric acid	15063213	1
Caesar&Loretz GmbH	Citric acid	16038604	1
Caesar&Loretz GmbH	Citric acid	22000645001	1
Caesar&loretz,Phoenix	Citric acid	13243201	1
Caesar&Loretz/Geilen...	Citric acid	18312104	1
Caesar/Lorenz	Citric acid	13050610	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caleo/ Noweda	Citric acid	18097607	1
Caleo/Fiebig	Citric acid	18025704	1
Caleo	Citric acid	16038613	1
Caolo- Noweda	Citric acid	15063213	1
Cealo / Otto Geilenk...	Citric acid	18306909	1
Cealo/AHD	Citric acid	16038704	1
Cealo/Anzag	Citric acid	16208607	1
Cealo/Gehe	Citric acid	14186301	6
Cealo/Sanacorp	Citric acid	17329502	1
Cealo	Citric acid	16004701	1
Cordes/Noweda	Citric acid	16208607	1
E Plus	Citric acid	16208613	1
Ebert & Jacobi 12...	Citric acid	1506214	1
Ebert & Jacobi	Citric acid	16215403	1
Ebert & Jacobi	Citric acid	6493071	1
Ebert-Jacobi	Citric acid	16208607	1
Eu Rho	Citric acid	L1202001-01	1
EuRho/Alliance Healthcare	Citric acid	L1609021-02	1
EuRho/Phönix	Citric acid	L1408011-02	1
EuRho	Citric acid	L1503027-02	2
euro / Phoenix 19.02.2018	Citric acid	11609021	1
Euro OTC	Citric acid		4
Euro OTC	Citric acid	1011047-03	2
Euro OTC	Citric acid	1018M-01024	1
Euro OTC	Citric acid	1018M-0124	1
Euro OTC	Citric acid	1275983	2
Euro OTC	Citric acid	13175410	1
Euro OTC	Citric acid	13396515	1
Euro OTC	Citric acid	13K18-B34	1
Euro OTC	Citric acid	1406014-02	1
Euro OTC	Citric acid	150317-965	1
Euro OTC	Citric acid	1505029B	1
Euro OTC	Citric acid	16004702	1
Euro OTC	Citric acid	16038713	1
Euro OTC	Citric acid	17162601	2
Euro OTC	Citric acid	17329502	1
Euro OTC	Citric acid	2112002-01	1
Euro OTC	Citric acid	2301021-01	1
Euro OTC	Citric acid	702260	5
Euro OTC	Citric acid	Intern-Ch1018M-01024	1
Euro OTC	Citric acid	L1202001-01	5
Euro OTC	Citric acid	L1202001-02	1
Euro OTC	Citric acid	L130404201	2
Euro OTC	Citric acid	L1304042-01	2
Euro OTC	Citric acid	L1304042-02	1
Euro OTC	Citric acid	L1408011-01	2
Euro OTC	Citric acid	L1408011-02	2
Euro OTC	Citric acid	L1503027-01	1
Euro OTC	Citric acid	L1503027-02	5
Euro OTC	Citric acid	L1508013-01	4
Euro OTC	Citric acid	L1508013-02	1
Euro OTC	Citric acid	L1604061-02	5
Euro OTC	Citric acid	l1604062-01	1
Euro OTC	Citric acid	L160461-02	1
Euro OTC	Citric acid	L1609021-01	6
Euro OTC	Citric acid	L1609021-02	4
Euro OTC	Citric acid	L1805017-01	2
Euro OTC	Citric acid	L1812017-01	5
Euro OTC	Citric acid	L1812017-02	1
Euro OTC	Citric acid	L2002036-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Citric acid	L2002036-02	1
Euro OTC	Citric acid	L2010013-01	1
Fagron	Citric acid		1
Fagron	Citric acid	100614d	1
Fagron	Citric acid	10G21-N05	2
Fagron	Citric acid	1151608	2
Fagron	Citric acid	1155609	9
Fagron	Citric acid	1156158	1
Fagron	Citric acid	1172673	10
Fagron	Citric acid	1181765	3
Fagron	Citric acid	11C24-N02	3
Fagron	Citric acid	11C24N022869/4250	1
Fagron	Citric acid	11C24-N03	6
Fagron	Citric acid	11H30-N05	1
Fagron	Citric acid	11K07N01	1
Fagron	Citric acid	11K07-N01	7
Fagron	Citric acid	11K11-N02	2
Fagron	Citric acid	11K11-N020444/1975	1
Fagron	Citric acid	12175711	1
Fagron	Citric acid	12801-N01	1
Fagron	Citric acid	12b01-N01	1
Fagron	Citric acid	12B01N01	1
Fagron	Citric acid	12B01-N01	23
Fagron	Citric acid	12B01-No1	1
Fagron	Citric acid	12B01-NO1	1
Fagron	Citric acid	12BO1-N01	1
Fagron	Citric acid	12F06-M06	3
Fagron	Citric acid	13804-N02	1
Fagron	Citric acid	13A04N04	1
Fagron	Citric acid	13A04-N04	13
Fagron	Citric acid	13A-04-N04	2
Fagron	Citric acid	13A04-N040019/4900	1
Fagron	Citric acid	13A04-NO4	1
Fagron	Citric acid	13B04-N01	1
Fagron	Citric acid	13F12-N01	3
Fagron	Citric acid	13F12-N08	1
Fagron	Citric acid	13G04-N05	5
Fagron	Citric acid	13G24-N13	6
Fagron	Citric acid	13G24-N24	13
Fagron	Citric acid	13G24-N240029/900	1
Fagron	Citric acid	13G24-N240739/900	1
Fagron	Citric acid	13H22-N09	2
Fagron	Citric acid	13K18-B34	5
Fagron	Citric acid	13K18-B34_291522	1
Fagron	Citric acid	13K18-B34-288371	4
Fagron	Citric acid	13k18-B34-288372	1
Fagron	Citric acid	13K18-B34-288372	7
Fagron	Citric acid	13K18-B34-288373	1
Fagron	Citric acid	13K18-B34-291071	4
Fagron	Citric acid	13K18-B34-291072	2
Fagron	Citric acid	13K18-B34-291519	5
Fagron	Citric acid	13K18-B34-291520	4
Fagron	Citric acid	13K18-B34-291521	4
Fagron	Citric acid	13k18-b34-291522	1
Fagron	Citric acid	13K18-B34-291522	6
Fagron	Citric acid	13K18-B34-291523	2
Fagron	Citric acid	13K18-B34-293871	2
Fagron	Citric acid	13L05-B02-296246	3
Fagron	Citric acid	13L05B02296247	1
Fagron	Citric acid	13L05-B02-309050	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Citric acid	13L18-B39-289347	4
Fagron	Citric acid	14b06-b07-293872	1
Fagron	Citric acid	14E06-B07293872	1
Fagron	Citric acid	14E06-B07-293872	4
Fagron	Citric acid	14E06-B07293873	1
Fagron	Citric acid	14E06-B07-293873	1
Fagron	Citric acid	14E06-B07-293875	3
Fagron	Citric acid	14E06-B07-293890	4
Fagron	Citric acid	14E-06-B07-293890	1
Fagron	Citric acid	14G04-B09-293874	11
Fagron	Citric acid	14G04-b09-293876	1
Fagron	Citric acid	14G04B09293876	1
Fagron	Citric acid	14G04-B09-293876	4
Fagron	Citric acid	14g04-b09293877	1
Fagron	Citric acid	14G04-B09-293877	12
Fagron	Citric acid	14G04-B09-296361	1
Fagron	Citric acid	14G04-B09-309707	1
Fagron	Citric acid	14G04-B09-309836	3
Fagron	Citric acid	14K05_B04_302815	1
Fagron	Citric acid	14K05-B04-302815	6
Fagron	Citric acid	14k05-b04-302816	1
Fagron	Citric acid	14K05-B04-302816	6
Fagron	Citric acid	14K05-B04-302817	2
Fagron	Citric acid	14K05-B04-302826	1
Fagron	Citric acid	15044902	1
Fagron	Citric acid	15G16b01	1
Fagron	Citric acid	15G16B01	1
Fagron	Citric acid	15G16-B01	2
Fagron	Citric acid	15G16-B01330449	2
Fagron	Citric acid	15G16-B01-330449	16
Fagron	Citric acid	15g16-b01-330450	2
Fagron	Citric acid	15G16B01330450	1
Fagron	Citric acid	15G16-B01330450	1
Fagron	Citric acid	15G16-B01-330450	8
Fagron	Citric acid	15G16-B01-330450	1
Fagron	Citric acid	15l01-B06-324348	1
Fagron	Citric acid	16072014B	1
Fagron	Citric acid	16208607	1
Fagron	Citric acid	1714Q1024	1
Fagron	Citric acid	17E15-B04	2
Fagron	Citric acid	17E15-B04-335435	3
Fagron	Citric acid	17E15-B04-341741	1
Fagron	Citric acid	17E15-B04-345678	6
Fagron	Citric acid	17E15-B04-345679	3
Fagron	Citric acid	17E15-B04-347168	3
Fagron	Citric acid	17E15-B04-347169	3
Fagron	Citric acid	18F25-B02	1
Fagron	Citric acid	18F25-B02-351448	1
Fagron	Citric acid	18F25-B02-351454	1
Fagron	Citric acid	18F25-B02-355281	3
Fagron	Citric acid	18F25-B02-355298	2
Fagron	Citric acid	1913A-01024	1
Fagron	Citric acid	19B06-B02-191458	1
Fagron	Citric acid	19h23-B07-194438	1
Fagron	Citric acid	19H23-B07-194438	4
Fagron	Citric acid	19H23B07194441	1
Fagron	Citric acid	19H23-B07-200458	1
Fagron	Citric acid	19H23-Bo7-200458	1
Fagron	Citric acid	20071203	1
Fagron	Citric acid	20F16-B02-201199	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Citric acid	20G31-B01-201878	3
Fagron	Citric acid	20L01-B10-202958	2
Fagron	Citric acid	214U-01024	1
Fagron	Citric acid	21F00-B04-218885	1
Fagron	Citric acid	21F11-804-218885	1
Fagron	Citric acid	21F11-B03-216679	1
Fagron	Citric acid	21F11-B04-213768	2
Fagron	Citric acid	21F11-B04-218885	2
Fagron	Citric acid	21F11-B04-221484	1
Fagron	Citric acid	2203140l	1
Fagron	Citric acid	22G15-B05-220815	1
Fagron	Citric acid	26082013B	1
Fagron	Citric acid	28021404	1
Fagron	Citric acid	2OF16-BO2_201199	1
Fagron	Citric acid	330449	1
Fagron	Citric acid	351453	1
Fagron	Citric acid	4810E-01024	1
Fagron	Citric acid	6496091	1
Fagron	Citric acid	700309-0001	1
Fagron	Citric acid	700309-0003	2
Fagron	Citric acid	700309-0006	1
Fagron	Citric acid	700309-001	1
Fagron	Citric acid	7200458	1
Fagron	Citric acid	L1604061-02	1
Fagron	Citric acid	L1812017-01	2
Fagron	Citric acid	probe	1
Fagron	Citric acid	UJ051	1
Fagron	Citric acid	UJ501	2
Fargon/Sanacorp	Citric acid		1
Fargon	Citric acid	12B01-N01	1
Fargon	Citric acid	12B01-NN01	1
fargon	Citric acid	13A04-N04	1
Faron	Citric acid	UJ45	1
Fiebig	Citric acid	13243201	1
Fiebig	Citric acid	14K05-B04-302815	1
Fiebig	Citric acid	15063204	1
Fiebig	Citric acid	17162702	1
Finze	Citric acid	12156812	2
Fischar/Noweda	Citric acid	6494061	1
Fischar/Phönix	Citric acid	6497051	2
Fischar	Citric acid	649061	2
fischar	Citric acid	6491041	1
Fischar	Citric acid	6493071	1
Fischar	Citric acid	6494061	2
Fischar	Citric acid	6496091	2
Fischar	Citric acid	6498011	2
Fischar	Citric acid	6499061	1
Fischer/Noweda	Citric acid	6496091	1
fishar	Citric acid	6494061	1
Fragon/Phoenix	Citric acid	14G04-B09-293976	1
Fragon/Phönix	Citric acid	18F25-B02-351463	1
Fragron/Noweda	Citric acid	15G16-B01-330449	1
GEHE 02.07.2014	Citric acid	13243217	1
Gehe 21-01-2019	Citric acid	18097609	1
Gehe amax	Citric acid	18129205	1
Gehe amax	Citric acid	192036003	1
Gehe Kassel, 22.05.2015	Citric acid	14E06-B07-293872	1
Gehe Rostock	Citric acid	21000543006	1
Gehe/Euro	Citric acid	160406-02	1
Gehe/Fragon	Citric acid	14G04B09293876	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Citric acid	11C24-N02	1
Gehe	Citric acid	11C24-N03	2
Gehe	Citric acid	11K07-N01	2
Gehe	Citric acid	12043111	1
Gehe	Citric acid	13175403	1
Gehe	Citric acid	13175404	1
Gehe	Citric acid	15044902	1
Gehe	Citric acid	15063003	1
Gehe	Citric acid	15063203	1
Gehe	Citric acid	15063217	1
Gehe	Citric acid	15087902	1
Gehe	Citric acid	15G16-B01-330450	1
Gehe	Citric acid	16004706	1
Gehe	Citric acid	16038614	1
GEHE	Citric acid	16208606	1
Gehe	Citric acid	16208612	1
Gehe	Citric acid	17162601	2
Gehe	Citric acid	17162602	1
Gehe	Citric acid	17162603	1
Gehe	Citric acid	18097607	1
GEHE	Citric acid	18097607	1
GEHE	Citric acid	18097611	1
Gehe	Citric acid	18306906	1
Gehe	Citric acid	18307102	1
Gehe	Citric acid	192073009	1
Gehe	Citric acid	20000886003	1
Gehe	Citric acid	21000544001	1
Gehe	Citric acid	21002657003	1
GEHE	Citric acid	21002657003	1
Gehe	Citric acid	22000645011	1
GEHE	Citric acid	22000645011	1
Gehe	Citric acid	22002309001	1
Geilenkirchen	Citric acid	16208606	1
Geilenkirchen	Citric acid	18306906	1
Geilenkirchen	Citric acid	21000544002	1
Hedinger	Citric acid	18306906	1
Henry Lamotte Oils GmbH	Citric acid		1
Hepart	Citric acid	16208614	1
Ichthyol	Citric acid	16038608	1
Ichtyhol Gesellschaf...	Citric acid	16038618	1
Jenne 05.11.21 EK:6,97EUR	Citric acid	211108C	1
Jenne	Citric acid	15063002	1
Jenne	Citric acid	200000886007	1
Jungbunzlauer Ladenb...	Citric acid	1156158	1
Jungbunzlauer Ladenb...	Citric acid	1155609	1
Kehr.21.07.2020	Citric acid	192073004	1
Kehr.28.04.2020	Citric acid	192073005	2
Kehr	Citric acid	17162602	1
Kehr	Citric acid	22002250001	1
Kehr	Citric acid	22002309004	1
Klenk	Citric acid	12B01-N01	2
Klenk	Citric acid	13243201	1
Krieger	Citric acid	21002657015	1
L10	Citric acid	9494185	1
Lamotte	Citric acid	15063213	1
Merck	Citric acid		1
Merck	Citric acid	K53604941	1
Nachtestung-Verlängerung	Citric acid	278/18	1
Noweda 13.6.2019	Citric acid	18306905	2
Noweda	Citric acid	12043110	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Citric acid	13050601	1
Noweda	Citric acid	13050621	1
Noweda	Citric acid	13243216	1
Noweda	Citric acid	15063203	1
Noweda	Citric acid	15087902	2
Noweda	Citric acid	16004701	1
Noweda	Citric acid	16208606	3
Noweda	Citric acid	16208607	1
Noweda	Citric acid	16208614	1
Noweda	Citric acid	18025701	1
Noweda	Citric acid	18025704	1
Noweda	Citric acid	18097606	1
Noweda	Citric acid	18306903	1
Noweda	Citric acid	18306906	2
Noweda	Citric acid	18306911	1
Noweda	Citric acid	18307102	1
Noweda	Citric acid	18312104	1
Noweda	Citric acid	20000886002	1
Noweda	Citric acid	20000886009	1
Noweda	Citric acid	21000543008	1
Noweda	Citric acid	21000543010	1
Noweda	Citric acid	21002657003	1
Noweda	Citric acid	21002657015	2
Noweda	Citric acid	21002657016	1
Noweda	Citric acid	21002657017	1
Noweda	Citric acid	22000645001	1
Noweda	Citric acid	22000645005	1
Noweda	Citric acid	22002309004	1
Noweda	Citric acid	L1202001-02	1
O.Fischer GmbH/Anzag...	Citric acid	6498011	1
Otto Fischar GmbH&Co KG	Citric acid	6496091	1
Otto Fischar GmbH&Co. KG	Citric acid	6494061	6
Otto Fischar GmbH&Co. KG	Citric acid	6496051	1
Otto Fischar GmbH/ N...	Citric acid	6494061	1
Otto Fischar GmbH	Citric acid	6498011	1
Otto Fischar/Kehr	Citric acid	6498011	1
Otto Fischar	Citric acid	6494061	1
Otto Fischar	Citric acid	6498011	1
Otto Fischer / Sana	Citric acid	6493071	1
Otto Fischer GmbH & ...	Citric acid	6496091	1
Otto Fischer GmbH/Sana	Citric acid	6497051	1
Otto Fischer GmbH	Citric acid	6492061	1
Otto Fishar	Citric acid	6496091	2
Phoenix 07.04.2014	Citric acid	13A04-N04	1
Phoenix 12.12.2016 4,59EUR	Citric acid	1508808	1
Phoenix 14.08.2017	Citric acid	16038712	1
Phoenix 29.05.2019 2,48EUR	Citric acid	18306902	1
Phoenix 31.01.2019	Citric acid	18097607	1
phoenix 5.6.14	Citric acid	1172673	1
Phoenix	Citric acid	1172673	1
Phoenix	Citric acid	12b01-N01	1
Phoenix	Citric acid	13243202	1
Phoenix	Citric acid	13K18-B34-288372	1
Phoenix	Citric acid	16208606	1
Phoenix	Citric acid	16208614	1
Phoenix	Citric acid	18025701	1
Phoenix	Citric acid	18097603	1
Phoenix	Citric acid	18097607	1
Phoenix	Citric acid	18306911	1
Phoenix	Citric acid	19B06-B02-191458	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Citric acid	20000886009	1
Phoenix	Citric acid	21000544002	2
Phoenix	Citric acid	21002657015	1
Phoenix	Citric acid	22000645011	1
Phoenix	Citric acid	22002309004	1
Phoenix	Citric acid	2310005-01	1
Phönix Gotha	Citric acid	12B01-N011973/6000	1
Phönix Gotha	Citric acid	12B01-N012028/6000	1
Phönix Gotha	Citric acid	12B01-N012125/6000	1
Phönix Gotha	Citric acid	13050609	1
Phönix Gotha	Citric acid	13050618	1
Phönix Gotha	Citric acid	13A04-N040049-100	1
Phönix Gotha	Citric acid	15063206	2
Phönix/Fagon	Citric acid	14604-B09-293876	1
Phönix/Gehe	Citric acid	16208614	1
Phönix	Citric acid	10005440022	1
Phönix	Citric acid	1155609	1
Phönix	Citric acid	123456	1
Phönix	Citric acid	13A04-N04	1
Phönix	Citric acid	14186312	4
Phönix	Citric acid	15063213	1
phönix	Citric acid	16038604	3
phönix	Citric acid	16208608	1
Phönix	Citric acid	16208613	1
Phönix	Citric acid	16215406	1
Phönix	Citric acid	18025702	2
Phönix	Citric acid	18025704	1
Phönix	Citric acid	18097601	1
Phönix	Citric acid	18097603	3
Phönix	Citric acid	18097607	1
Phönix	Citric acid	192073003	1
Phönix	Citric acid	192073005	1
Phönix	Citric acid	20000886002	1
Phönix	Citric acid	20000886003	1
Phönix	Citric acid	20000886009	1
Phönix	Citric acid	21000543002	1
Phönix	Citric acid	21000543011	1
Phönix	Citric acid	21000544004	1
Phönix	Citric acid	21002657003	1
Sanacorb;20.04.15; 7,45EUR	Citric acid	1375410	1
Sanacorp/Bionorica Ethics	Citric acid	16038622	1
Sanacorp	Citric acid	12156811	1
Sanacorp	Citric acid	12156823	1
Sanacorp	Citric acid	12156824	1
Sanacorp	Citric acid	12156832	1
Sanacorp	Citric acid	1216832	1
Sanacorp	Citric acid	13050604	1
Sanacorp	Citric acid	13243214	1
sanacorp	Citric acid	13396505	1
Sanacorp	Citric acid	13K18-B34-291072	1
Sanacorp	Citric acid	15i01-b06-324348	1
Sanacorp	Citric acid	16208608	1
Sanacorp	Citric acid	16208614	1
Sanacorp	Citric acid	17162601	5
Sanacorp	Citric acid	18025702	1
Sanacorp	Citric acid	18025704	1
Sanacorp	Citric acid	18097603	1
Sanacorp	Citric acid	183066905	1
Sanacorp	Citric acid	18306909	1
Sanacorp	Citric acid	192073004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Citric acid	192073005	1
Sanacorp	Citric acid	20000886002	1
Sanacorp	Citric acid	20003515003	1
Sanacorp	Citric acid	21000543011	3
Sanacorp	Citric acid	21000544001	1
Sanacorp	Citric acid	21002657015	2
Sanacorp	Citric acid	22000645004	1
Sanacorp	Citric acid	22002309001	2
Sanacorp	Citric acid	22002309004	1
Sanacorp	Citric acid	40/AKD2	1
Sanacorp	Citric acid	41/AKD4	1
SanacorpWE:15.02.201…	Citric acid	15063203	1
SanacorpWE:30.01.201…	Citric acid	16038707	1
Spangropharm	Citric acid	13050611	3
VDL 16.03.15; 2,54EUR	Citric acid	13243201	1
VDL;23.6.14; 2.49EUR	Citric acid	13243213	1
Wolf Apotheke	Citric acid	58(18097609)	1

- 231 724 spectra from 1513 *Apo-Ident* customers from a total of 48 608 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Citric acid* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Citric acid* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	1170	0	200 914
Type C	0	4319	24	231 724

The substance/substance group *Citric acid* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4872 %)
Type C	100.0000 % (> 99.9007 %)	99.4474 % (> 99.3783 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20682	22463	20.26	98.56
20683	22463	5.50	111.16
20706	22463	19.43	99.00
20913	22463	5.43	123.72
21455	22463	23.26	97.83
21487	22463	14.74	103.95
22463	22463	0.00	118.38
26350	26350	0.00	114.01

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Citric acid monohydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20012-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Citric acid monohydrate; Acidum citricum monohydricum

Special notes

When selecting the *Citric acid monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Citric acid monohydrate	8	4	109

Second-stage model

For differentiation of the substance/substance group *Citric acid monohydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Citric acid monohydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	86.83	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Citric acid monohydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Citric acid monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Citric acid monohydrate	15185301	22340	60	20150708
Caelo	Citric acid monohydrate	17085602	23409	40	20170410
Caelo	Citric acid monohydrate	181305	24222	40	20180606*
Caelo	Citric acid monohydrate	19000762	25563	40	20200204*
Caelo	Citric acid monohydrate	23001973	26954	40	20231108*
Caelo	Citric acid monohydrate	23001973	26954SI	20	20231108*
Fagron	Citric acid monohydrate	12D26-N02	20926	40	20120515
Hedinger	Citric acid monohydrate	202029	23457	40	20161110
Hedinger	Citric acid monohydrate	202029	23458	40	1908675
Hedinger	Citric acid monohydrate	202030	24874	40	20180727

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 400 spectra of 10 reference samples from the substance/substance group *Citric acid monohydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 562 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 250 spectra of 7 reference samples from the substance/substance group *Citric acid monohydrate*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Citric acid monohydrate	161865	22617	40
Caelo	Citric acid monohydrate	21001368	25796	50
Caelo	Citric acid monohydrate	22001438	26121	40
Caelo	Citric acid monohydrate	23001974	26948	40
Caelo	Citric acid monohydrate	161865	23298	40
Caelo	Citric acid monohydrate	22001438	26121SI	20
Caelo	Citric acid monohydrate	23001974	26948SI	20

- 201 834 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 409 spectra from 186 *Apo-Ident* customers from 113 batches from the substance/substance group *Citric acid monohydrate*.

- Among them are spectra of independent samples from 105 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Citric acid monohydrate	22001438007	4
AEP	Citric acid monohydrate	190884005	1
AHD	Citric acid monohydrate	22001438007	2
AHD	Citric acid monohydrate	23003303002	1
Alliance Healthcare	Citric acid monohydrate	18130503	1
Bombastus	Citric acid monohydrate		1
Bombastus	Citric acid monohydrate	18000110	1
Bombastus	Citric acid monohydrate	18003283	1
Bombastus	Citric acid monohydrate	18003407	1
Bombastus	Citric acid monohydrate	201-069-1	2
Bombastus	Citric acid monohydrate	259437	1
Bombastus	Citric acid monohydrate	294630	1
Bombastus	Citric acid monohydrate	309343	1
Bombastus	Citric acid monohydrate	309344	2
Bombastus	Citric acid monohydrate	309650	1
Bombastus	Citric acid monohydrate	310803	2
Bombastus	Citric acid monohydrate	70620101	1
Caelo	Citric acid monohydrate	11208132	3
Caelo	Citric acid monohydrate	11208133	4
Caelo	Citric acid monohydrate	12125904	2
Caelo	Citric acid monohydrate	12125907	6
Caelo	Citric acid monohydrate	12125937	3
Caelo	Citric acid monohydrate	12125938	1
Caelo	Citric acid monohydrate	1212937	1
Caelo	Citric acid monohydrate	1215907	1
Caelo	Citric acid monohydrate	1215911	1
Caelo	Citric acid monohydrate	13069103	1
Caelo	Citric acid monohydrate	13069104	6
Caelo	Citric acid monohydrate	13069105	2
Caelo	Citric acid monohydrate	13069106	3
Caelo	Citric acid monohydrate	13069110	4
Caelo	Citric acid monohydrate	13069111	3
Caelo	Citric acid monohydrate	13069113	2
Caelo	Citric acid monohydrate	13069124	4
Caelo	Citric acid monohydrate	13069125	2
Caelo	Citric acid monohydrate	13069128	3
Caelo	Citric acid monohydrate	13069129	4
Caelo	Citric acid monohydrate	13069130	1
Caelo	Citric acid monohydrate	13069133	5
Caelo	Citric acid monohydrate	14038401	6
Caelo	Citric acid monohydrate	14038403	8
Caelo	Citric acid monohydrate	14071701	1
Caelo	Citric acid monohydrate	14311807	2
Caelo	Citric acid monohydrate	14311808	4
Caelo	Citric acid monohydrate	14311812	4
Caelo	Citric acid monohydrate	14311813	1
Caelo	Citric acid monohydrate	15087502	2
Caelo	Citric acid monohydrate	15087503	2
Caelo	Citric acid monohydrate	15087509	9
Caelo	Citric acid monohydrate	15087510	2
Caelo	Citric acid monohydrate	15087512	1
Caelo	Citric acid monohydrate	15185301	2
Caelo	Citric acid monohydrate	15185302	14
Caelo	Citric acid monohydrate	15185304	12
Caelo	Citric acid monohydrate	15185309	5
Caelo	Citric acid monohydrate	15185314	5
Caelo	Citric acid monohydrate	15185316	6
Caelo	Citric acid monohydrate	15185317	2
Caelo	Citric acid monohydrate	15185320	3
Caelo	Citric acid monohydrate	15185321	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Citric acid monohydrate	161865001	1
Caelo	Citric acid monohydrate	16186501	5
Caelo	Citric acid monohydrate	16186502	6
Caelo	Citric acid monohydrate	16186508	6
Caelo	Citric acid monohydrate	17085602	9
Caelo	Citric acid monohydrate	17085603	8
Caelo	Citric acid monohydrate	17085607	5
Caelo	Citric acid monohydrate	17329801	1
Caelo	Citric acid monohydrate	17329804	16
Caelo	Citric acid monohydrate	17329807	1
Caelo	Citric acid monohydrate	17329808	4
Caelo	Citric acid monohydrate	18130503	3
Caelo	Citric acid monohydrate	18130506	1
Caelo	Citric acid monohydrate	18130509	1
Caelo	Citric acid monohydrate	18130510	2
Caelo	Citric acid monohydrate	19000762002	4
Caelo	Citric acid monohydrate	1900762002	1
Caelo	Citric acid monohydrate	190884001	4
Caelo	Citric acid monohydrate	190884002	1
Caelo	Citric acid monohydrate	190884005	10
Caelo	Citric acid monohydrate	190884006	1
Caelo	Citric acid monohydrate	190884008	4
Caelo	Citric acid monohydrate	19088401	10
Caelo	Citric acid monohydrate	19088402	3
Caelo	Citric acid monohydrate	19088405	1
Caelo	Citric acid monohydrate	19088407	5
Caelo	Citric acid monohydrate	19088408	1
Caelo	Citric acid monohydrate	20003892007	2
Caelo	Citric acid monohydrate	20003892008	10
Caelo	Citric acid monohydrate	20003892012	1
Caelo	Citric acid monohydrate	21001368003	1
Caelo	Citric acid monohydrate	21001368006	11
Caelo	Citric acid monohydrate	21001368009	1
Caelo	Citric acid monohydrate	21001368010	2
Caelo	Citric acid monohydrate	21001368013	3
Caelo	Citric acid monohydrate	22001438003	4
Caelo	Citric acid monohydrate	22001438006	1
Caelo	Citric acid monohydrate	22001438007	1
Caelo	Citric acid monohydrate	2515Q-02959	1
Caelo	Citric acid monohydrate	2x19088400	1
Caelo	Citric acid monohydrate	9522496	1
Caelo	Citric acid monohydrate	sjdfksjfdkl	1
Caesar & Loretz GmbH…	Citric acid monohydrate	22001438003	1
Caesar & Loretz GmbH/Gehe	Citric acid monohydrate	19088401	1
Caesar & Loretz GmbH/Gehe	Citric acid monohydrate	22001438003	1
Caesar & Loretz GmbH…	Citric acid monohydrate	21001368006	1
Caesar & Loretz GmbH	Citric acid monohydrate	18130506	1
Caesar & Loretz GmbH	Citric acid monohydrate	19000762002	2
Caesar & Loretz GmbH	Citric acid monohydrate	190884001	2
Caesar & Loretz GmbH	Citric acid monohydrate	190884005	4
Caesar & Loretz GmbH	Citric acid monohydrate	190884008	1
Caesar & Loretz GmbH	Citric acid monohydrate	19088405	2
Caesar & Loretz GmbH	Citric acid monohydrate	19088407	3
Caesar & Loretz GmbH	Citric acid monohydrate	19088408	1
Caesar & Loretz GmbH	Citric acid monohydrate	20003892002	4
Caesar & Loretz GmbH	Citric acid monohydrate	20003892007	1
Caesar & Loretz GmbH	Citric acid monohydrate	20003892008	4
Caesar & Loretz GmbH	Citric acid monohydrate	2000392002	1
Caesar & Loretz GmbH	Citric acid monohydrate	21001368006	6
Caesar &Loretz GmbH	Citric acid monohydrate	12125937	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Cealo	Citric acid monohydrate	15185320	1
E Plus	Citric acid monohydrate	16186508	1
Ebert 17.08.16	Citric acid monohydrate	15185314	1
Euro OTC	Citric acid monohydrate	17085607	1
Europharm / Gehe	Citric acid monohydrate	17329804	1
Fiebig28.08.13 EK6,60	Citric acid monohydrate	13069111	1
Gehe	Citric acid monohydrate	17085602	1
Gehe	Citric acid monohydrate	17329804	1
Gehe	Citric acid monohydrate	22001438003	1
Gehe	Citric acid monohydrate	22001438007	1
Geilenkirchen	Citric acid monohydrate	16186502	1
Hänseler	Citric acid monohydrate		4
Hedinger / Phönix	Citric acid monohydrate	202029	1
Hedinger/Phönix	Citric acid monohydrate	202029	1
Hedinger	Citric acid monohydrate	202028	2
Hedinger	Citric acid monohydrate	202029	3
Henry Lamotte/AHD	Citric acid monohydrate	17329804	1
Herba Gatt Koller	Citric acid monohydrate	201103153211	1
Krieger	Citric acid monohydrate	613001-1-P	1
Nachprüfung	Citric acid monohydrate	AP201218-07	1
Phönix	Citric acid monohydrate	10111503	1
Phönix	Citric acid monohydrate	1403/3	1
Sanacaorp	Citric acid monohydrate	14038401	2
Sanacorp	Citric acid monohydrate	1215937	1
Sanacorp	Citric acid monohydrate	21001368006	1
Sanacorp	Citric acid monohydrate	22001438007	1
VDL	Citric acid monohydrate	263669	1

- 235 658 spectra from 1515 *Apo-Ident* customers from a total of 49 149 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Citric acid monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Citric acid monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	250	0	201 834
Type C	0	406	3	235 658

The substance/substance group *Citric acid monohydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.6000 %)
Type C	100.0000 % (> 99.9007 %)	99.2665 % (> 98.5330 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20926	23458	6.98	226.73
22340	26954	13.90	225.59
23409	23458	11.58	227.97
23457	26954	9.19	226.71
23458	23458	0.00	226.97
24222	24222	0.00	228.98
24874	26954	5.13	225.98
25563	25563	0.00	226.69
26954	26954	0.00	223.67

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Citrulline**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21095-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Citrulline; Citrullinum; L-citrulline

Special notes

When selecting the *Citrulline* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Citrulline	9	11	22

Second-stage model

For differentiation of the substance/substance group *Citrulline* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Citrulline* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	93.45	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Citrulline* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Citrulline*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Citrulline	1310015-01	21095	40	20131120
Euro OTC	Citrulline	1403021-01	21565	59	1411031
Euro OTC	Citrulline	1604038	22560	40	20160523*
Euro OTC	Citrulline	1703036	23175	40	20170418*
Euro OTC	Citrulline	1811028	24348	40	20181127*
Euro OTC	Citrulline	2003033	25415	40	20200914*
Euro OTC	Citrulline	2011009	25462	40	20201126*
Fagron	Citrulline	16D11-B02-326797	23567	40	20160421
Fagron	Citrulline	18K15-B01-356962	24643	40	20190123

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 379 spectra of 9 reference samples from the substance/substance group *Citrulline*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 583 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 510 spectra of 14 reference samples from the substance/substance group *Citrulline*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Citrulline	1609013	22866	40
Euro OTC	Citrulline	1707003	23538	40
Euro OTC	Citrulline	1710039	23913	40
Euro OTC	Citrulline	1805028	24117	40
Euro OTC	Citrulline	1904013	24627	40
Euro OTC	Citrulline	2001002	25070	40
Euro OTC	Citrulline	2109012	25827	50
Euro OTC	Citrulline	2301010	26517	40
Euro OTC	Citrulline	2401009	27163	40
Fagron	Citrulline	19E03-B01-362002	24819	40
Fagron	Citrulline	22G22-B05-222418	26375	40
Euro OTC	Citrulline	2301010	26517SI	20
Euro OTC	Citrulline	2401009	27163SI	20
Fagron	Citrulline	22G22-B05-222418	26375SI	20

- 201 574 spectra from a total of 4034 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 32 spectra from 9 *Apo-Ident* customers from 23 batches from the substance/substance group *Citrulline*.

- Among them are spectra of independent samples from 20 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Citrulline	17C14-B01-339452	2
Dr. Schär	Citrulline	R1216-022A	1
Dr.Schär GmbH (Direkt)	Citrulline	20190700	1
Dr.Schär GmbH (Direkt)	Citrulline	20200027	1
Euro OTC	Citrulline	16040038-01	1
Euro OTC	Citrulline	1811028-01	1
Euro OTC	Citrulline	1904013-01	2
Euro OTC	Citrulline	2001002-01	3
Euro OTC	Citrulline	20011002-01	1
Euro OTC	Citrulline	2003033-01	3
Euro OTC	Citrulline	2011009-01	2
Euro OTC	Citrulline	2109012-01	1
Euro OTC	Citrulline	CIT-PL-19102	1
Fagron	Citrulline	18B12-B02	1
Fagron	Citrulline	18K15-B01	1
Fagron	Citrulline	19M17F01366482	1
Fagron	Citrulline	20A28-F02-368558	1
Fagron	Citrulline	21C08-F05-377311	2
Gall-Pharma GmbH/Noweda	Citrulline		1
Gall-Pharma GmbH	Citrulline		1
Hecht-Pharma/ Noweda	Citrulline		1
Nutricia	Citrulline	100803609	1
Nutricia	Citrulline	100915050	2

- 236 035 spectra from 1515 *Apo-Ident* customers from a total of 49 236 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Citrulline* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Citrulline* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	379	0	152 583
Type B	0	510	0	201 574
Type C	0	31	1	236 035

The substance/substance group *Citrulline* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4169 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8235 %)
Type C	100.0000 % (> 99.9007 %)	96.8750 % (> 87.5000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21095	21565	9.88	131.20
21565	21565	0.00	127.86
22560	22560	0.00	138.37
23175	23175	0.00	142.33
23567	22560	4.78	140.79
24348	24348	0.00	126.86
24643	25462	5.50	137.08
25415	25415	0.00	144.00
25462	25462	0.00	136.47

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Clindamycin hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20214-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Clindamycin hydrochloride; Clindamycini hydrochloridum

Special notes

When selecting the *Clindamycin hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Clindamycin hydrochloride	11	13	324

Second-stage model

For differentiation of the substance/substance group *Clindamycin hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Clindamycin hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	46.40	–
Colistin sulfate	63.21	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Clindamycin hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Clindamycin hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Clindamycin hydrochloride	15392809	22958	40	20151204
Caelo	Clindamycin hydrochloride	15392817	23245	40	20151204
Caelo	Clindamycin hydrochloride	21000113013	25927	40	20210212
Caelo	Clindamycin hydrochloride	21000113013	25927SI	40	20210212
Euro OTC	Clindamycin hydrochloride	1111058-01	20757	80	20120516
Euro OTC	Clindamycin hydrochloride	1511004	21996	60	20151123*
Euro OTC	Clindamycin hydrochloride	1510038	22224	60	20151120*
Euro OTC	Clindamycin hydrochloride	2001044	25074	40	20200303*
Euro OTC	Clindamycin hydrochloride	2004001	25307	40	20200804*
Euro OTC	Clindamycin hydrochloride	2004001	25307SI	40	20200804*
Fagron	Clindamycin hydrochloride	13G24-N09	21224	40	1412075
Fagron	Clindamycin hydrochloride	16D05-B08-332106	23264	40	20160504
Fagron	Clindamycin hydrochloride	24A23-B01-003404	27423	40	20240304
Fagron	Clindamycin hydrochloride	24A23-B01-003404	27423SI	40	20240304

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 640 spectra of 14 reference samples from the substance/substance group *Clindamycin hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 322 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 790 spectra of 20 reference samples from the substance/substance group *Clindamycin hydrochloride*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Clindamycin hydrochloride	153928	23365	40
Caelo	Clindamycin hydrochloride	172093	23681	40
Caelo	Clindamycin hydrochloride	22001232	26128	30
Caelo	Clindamycin hydrochloride	23003574	27135	40
Euro OTC	Clindamycin hydrochloride	1401041-01	21239	40
Euro OTC	Clindamycin hydrochloride	1710013	23769	40
Euro OTC	Clindamycin hydrochloride	1811003	24336	40
Euro OTC	Clindamycin hydrochloride	1903009	24637	40
Euro OTC	Clindamycin hydrochloride	2201043	25949	40
Euro OTC	Clindamycin hydrochloride	2208011	26341	40
Euro OTC	Clindamycin hydrochloride	2307031	26875	40
Euro OTC	Clindamycin hydrochloride	2410002	27452	40
Fagron	Clindamycin hydrochloride	23B24-B05-231501	26825	40
Caelo	Clindamycin hydrochloride	22001232	26128SI	40
Caelo	Clindamycin hydrochloride	23003574	27135SI	40
Euro OTC	Clindamycin hydrochloride	2201043	25949SI	40
Euro OTC	Clindamycin hydrochloride	2208011	26341SI	40
Euro OTC	Clindamycin hydrochloride	2307031	26875SI	40
Euro OTC	Clindamycin hydrochloride	2410002	27452SI	40
Fagron	Clindamycin hydrochloride	23B24-B05-231501	26825SI	40

- 201 294 spectra from a total of 4032 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1085 spectra from 377 *Apo-Ident* customers from 336 batches from the substance/substance group *Clindamycin hydrochloride*.

- Among them are spectra of independent samples from 324 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Clindamycin hydrochloride	22001232004	2
	Clindamycin hydrochloride	22001232007	1
	Clindamycin hydrochloride	22001232008	7
	Clindamycin hydrochloride	22001232009	1
	Clindamycin hydrochloride	2208011-01	3
	Clindamycin hydrochloride	22A31-F04-383139	2
	Clindamycin hydrochloride	22A31-F04-382350	1
	Clindamycin hydrochloride	22G06-F01-383254	2
	Clindamycin hydrochloride	22G06-F01-383866	1
	Clindamycin hydrochloride	22G06-F01-383867	2
	Clindamycin hydrochloride	23003574001	2
	Clindamycin hydrochloride	23003574003	1
	Clindamycin hydrochloride	23B24-B05-235823	2
	Clindamycin hydrochloride	F0138325004	1
	Clindamycin hydrochloride	F01-3843600	2
	Clindamycin hydrochloride	F01-3843602	1
34543453	Clindamycin hydrochloride	5345435345	1
adfgafda	Clindamycin hydrochloride	dsgadgadfg	1
AHD	Clindamycin hydrochloride	130402X5	1
AHD	Clindamycin hydrochloride	16H03-B02-343063	1
AHD	Clindamycin hydrochloride	1710013-01	1
AHD	Clindamycin hydrochloride	23003574002	1
Anzag	Clindamycin hydrochloride	15392815	1
Bombastus	Clindamycin hydrochloride	1710013-01	1
Caelo	Clindamycin hydrochloride		1
Caelo	Clindamycin hydrochloride	10809406	1
Caelo	Clindamycin hydrochloride	1111058-03	1
Caelo	Clindamycin hydrochloride	11K04-N12	1
Caelo	Clindamycin hydrochloride	13G24-N09	1
Caelo	Clindamycin hydrochloride	1401041-01	2
Caelo	Clindamycin hydrochloride	140104102	1
Caelo	Clindamycin hydrochloride	14K04B05309851	1
Caelo	Clindamycin hydrochloride	151003801	2
Caelo	Clindamycin hydrochloride	1511004-01	3
Caelo	Clindamycin hydrochloride	1511004-02	1
Caelo	Clindamycin hydrochloride	1511004-03	2
Caelo	Clindamycin hydrochloride	15189512	1
Caelo	Clindamycin hydrochloride	15392802	1
Caelo	Clindamycin hydrochloride	15392804	4
Caelo	Clindamycin hydrochloride	15392805	1
Caelo	Clindamycin hydrochloride	15392807	1
Caelo	Clindamycin hydrochloride	15392811	2
Caelo	Clindamycin hydrochloride	15392814	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clindamycin hydrochloride	15392815	4
Caelo	Clindamycin hydrochloride	15392816	1
Caelo	Clindamycin hydrochloride	15392817	3
Caelo	Clindamycin hydrochloride	15392818	2
Caelo	Clindamycin hydrochloride	15392819	1
Caelo	Clindamycin hydrochloride	15392822	2
Caelo	Clindamycin hydrochloride	15E06-B12-310472	1
Caelo	Clindamycin hydrochloride	15L22-B03-318788	1
Caelo	Clindamycin hydrochloride	160712C	2
Caelo	Clindamycin hydrochloride	16d05-b08-332106	1
Caelo	Clindamycin hydrochloride	16H03-B02	1
Caelo	Clindamycin hydrochloride	16H03-B02-336706	1
Caelo	Clindamycin hydrochloride	16H03-B02-339275	1
Caelo	Clindamycin hydrochloride	16H03-B03-334345	1
Caelo	Clindamycin hydrochloride	17001301	1
Caelo	Clindamycin hydrochloride	17209301	2
Caelo	Clindamycin hydrochloride	17209302	3
Caelo	Clindamycin hydrochloride	17209303	3
Caelo	Clindamycin hydrochloride	180009408	1
Caelo	Clindamycin hydrochloride	18009401	3
Caelo	Clindamycin hydrochloride	18009402	2
Caelo	Clindamycin hydrochloride	18009403	5
Caelo	Clindamycin hydrochloride	18009405	4
Caelo	Clindamycin hydrochloride	18009406	3
Caelo	Clindamycin hydrochloride	18009408	1
Caelo	Clindamycin hydrochloride	18009409	5
Caelo	Clindamycin hydrochloride	18009410	1
Caelo	Clindamycin hydrochloride	18009412	6
Caelo	Clindamycin hydrochloride	18009413	2
Caelo	Clindamycin hydrochloride	18009414	3
Caelo	Clindamycin hydrochloride	18009416	4
Caelo	Clindamycin hydrochloride	1811003-01	3
Caelo	Clindamycin hydrochloride	18A18-B08-346106	2
Caelo	Clindamycin hydrochloride	18A18-B08-346107	1
Caelo	Clindamycin hydrochloride	18D11-B01-349677	1
Caelo	Clindamycin hydrochloride	18J15-B04-355581	2
Caelo	Clindamycin hydrochloride	18J15-B04-358084	1
Caelo	Clindamycin hydrochloride	1903009-01	2
Caelo	Clindamycin hydrochloride	191332001	1
Caelo	Clindamycin hydrochloride	191392001	3
Caelo	Clindamycin hydrochloride	191392003	1
Caelo	Clindamycin hydrochloride	19139201	4
Caelo	Clindamycin hydrochloride	19139202	14
Caelo	Clindamycin hydrochloride	19139203	8
Caelo	Clindamycin hydrochloride	193087001	4
Caelo	Clindamycin hydrochloride	193087003	7
Caelo	Clindamycin hydrochloride	193087005	2
Caelo	Clindamycin hydrochloride	20001357001	3
Caelo	Clindamycin hydrochloride	20001357002	6
Caelo	Clindamycin hydrochloride	20001357003	3
Caelo	Clindamycin hydrochloride	20001357004	2
Caelo	Clindamycin hydrochloride	20001357005	7
Caelo	Clindamycin hydrochloride	20001357006	1
Caelo	Clindamycin hydrochloride	200035705	1
Caelo	Clindamycin hydrochloride	20004499001	3
Caelo	Clindamycin hydrochloride	20004499002	3
Caelo	Clindamycin hydrochloride	2072002	1
Caelo	Clindamycin hydrochloride	2100011300	1
Caelo	Clindamycin hydrochloride	21000113002	10
Caelo	Clindamycin hydrochloride	21000113003	6

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clindamycin hydrochloride	21000113004	1
Caelo	Clindamycin hydrochloride	21000113005	1
Caelo	Clindamycin hydrochloride	21000113006	3
Caelo	Clindamycin hydrochloride	21000113007	8
Caelo	Clindamycin hydrochloride	21000113008	2
Caelo	Clindamycin hydrochloride	21000113009	1
Caelo	Clindamycin hydrochloride	21000113010	1
Caelo	Clindamycin hydrochloride	21000113011	2
Caelo	Clindamycin hydrochloride	21000113012	1
Caelo	Clindamycin hydrochloride	21000113013	8
Caelo	Clindamycin hydrochloride	21000113014	1
Caelo	Clindamycin hydrochloride	21000113015	1
Caelo	Clindamycin hydrochloride	2100113002	1
Caelo	Clindamycin hydrochloride	22001232002	1
Caelo	Clindamycin hydrochloride	22001232003	6
Caelo	Clindamycin hydrochloride	22001232008	1
Caelo	Clindamycin hydrochloride	3304	1
Caelo	Clindamycin hydrochloride	379/19AI	1
Caelo	Clindamycin hydrochloride	P-003-WS10100301	1
Caesar & Loretz GmbH...	Clindamycin hydrochloride	21000113005	1
Caesar & Loretz GmbH...	Clindamycin hydrochloride	19139202	1
Caesar & Loretz GmbH...	Clindamycin hydrochloride	19139203	1
Caesar & Loretz GmbH...	Clindamycin hydrochloride	21000113003	1
Caesar & Loretz GmbH/ E	Clindamycin hydrochloride	20004499002	1
Caesar & Loretz GmbH/Gehe	Clindamycin hydrochloride	193087003	1
Caesar & Loretz GmbH/Gehe	Clindamycin hydrochloride	22001232008	1
Caesar & Loretz GmbH...	Clindamycin hydrochloride	22001232004	1
Caesar & Loretz GmbH...	Clindamycin hydrochloride	20001357004	2
Caesar & Loretz GmbH...	Clindamycin hydrochloride	21000113004	1
Caesar & Loretz GmbH...	Clindamycin hydrochloride	F06-3643002	1
Caesar & Loretz GmbH...	Clindamycin hydrochloride	21000113004	1
Caesar & Loretz GmbH...	Clindamycin hydrochloride	21000113013	1
Caesar & Loretz GmbH...	Clindamycin hydrochloride	CN201810404	1
Caesar & Loretz GmbH	Clindamycin hydrochloride	191392001	2
CAESAR & LORETZ GMBH	Clindamycin hydrochloride	191392001	1
Caesar & Loretz GmbH	Clindamycin hydrochloride	19139201	2
Caesar & Loretz GmbH	Clindamycin hydrochloride	19139202	4
Caesar & Loretz GmbH	Clindamycin hydrochloride	19139203	2
Caesar & Loretz GmbH	Clindamycin hydrochloride	19190703	2
Caesar & Loretz GmbH	Clindamycin hydrochloride	193087001	2
Caesar & Loretz GmbH	Clindamycin hydrochloride	193087002	1
Caesar & Loretz GmbH	Clindamycin hydrochloride	193087003	5
Caesar & Loretz GmbH	Clindamycin hydrochloride	193087004	2
Caesar & Loretz GmbH	Clindamycin hydrochloride	19H28-F06-3643002	1
Caesar & Loretz GmbH	Clindamycin hydrochloride	20001357001	2
Caesar & Loretz GmbH	Clindamycin hydrochloride	20001357002	3
Caesar & Loretz GmbH	Clindamycin hydrochloride	20001357003	2
Caesar & Loretz GmbH	Clindamycin hydrochloride	20001357004	1
Caesar & Loretz GmbH	Clindamycin hydrochloride	20001357005	2
Caesar & Loretz GmbH	Clindamycin hydrochloride	20004499001	1
Caesar & Loretz GmbH	Clindamycin hydrochloride	20004499003	2
Caesar & Loretz GmbH	Clindamycin hydrochloride	21000113002	1
Caesar & Loretz GmbH	Clindamycin hydrochloride	21000113003	2
Caesar & Loretz GmbH	Clindamycin hydrochloride	21000113004	1
Caesar & Loretz GmbH	Clindamycin hydrochloride	21000113005	1
Caesar & Loretz GmbH	Clindamycin hydrochloride	21000113006	1
Caesar & Loretz GmbH	Clindamycin hydrochloride	21000113007	2
Caesar & Loretz GmbH	Clindamycin hydrochloride	21000113010	1
Caesar & Loretz GmbH	Clindamycin hydrochloride	21000113011	3
Caesar & Loretz GmbH	Clindamycin hydrochloride	21000113012	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Clindamycin hydrochloride	21000113015	3
Caesar & Loretz GmbH	Clindamycin hydrochloride	2100013015	1
Caesar & Loretz GmbH	Clindamycin hydrochloride	22001232002	6
Caesar & Loretz GmbH	Clindamycin hydrochloride	22001232003	6
Caesar & Loretz GmbH	Clindamycin hydrochloride	22001232004	3
Caesar & Loretz GmbH	Clindamycin hydrochloride	F06-3661407	1
Caesar & Loretz Hilden	Clindamycin hydrochloride	18009401	1
Cealo/AHD	Clindamycin hydrochloride	16D05-B08-325088	1
Cealo	Clindamycin hydrochloride	1111058-01	1
EuRho/Noweda	Clindamycin hydrochloride	2201043-01	1
EuRho	Clindamycin hydrochloride	1401041-01	1
EuRho	Clindamycin hydrochloride	1710013-01	1
Euro OTC	Clindamycin hydrochloride	1111058-01	6
Euro OTC	Clindamycin hydrochloride	1111058-02	2
Euro OTC	Clindamycin hydrochloride	1111058-03	3
Euro OTC	Clindamycin hydrochloride	111158-01	1
Euro OTC	Clindamycin hydrochloride	130709X8	2
Euro OTC	Clindamycin hydrochloride	140104101	1
Euro OTC	Clindamycin hydrochloride	1401041-01	11
Euro OTC	Clindamycin hydrochloride	140104102	3
Euro OTC	Clindamycin hydrochloride	1401041-02	6
Euro OTC	Clindamycin hydrochloride	1401401-01	1
Euro OTC	Clindamycin hydrochloride	150714B	1
Euro OTC	Clindamycin hydrochloride	150901B	1
Euro OTC	Clindamycin hydrochloride	1510030-01	1
Euro OTC	Clindamycin hydrochloride	151003502	1
Euro OTC	Clindamycin hydrochloride	1510038-01	20
Euro OTC	Clindamycin hydrochloride	1510038-02	4
Euro OTC	Clindamycin hydrochloride	1511004-002	1
Euro OTC	Clindamycin hydrochloride	151100401	2
Euro OTC	Clindamycin hydrochloride	1511004-01	15
Euro OTC	Clindamycin hydrochloride	1511004-02	4
Euro OTC	Clindamycin hydrochloride	1511004-03	2
Euro OTC	Clindamycin hydrochloride	16D05-B08-328259	1
Euro OTC	Clindamycin hydrochloride	16H03-B02-334974	1
Euro OTC	Clindamycin hydrochloride	16H03-B02-339275	1
Euro OTC	Clindamycin hydrochloride	171001301	2
Euro OTC	Clindamycin hydrochloride	1710013-01	29
Euro OTC	Clindamycin hydrochloride	1710019-01	1
Euro OTC	Clindamycin hydrochloride	1811003-01	13
Euro OTC	Clindamycin hydrochloride	1903009	1
Euro OTC	Clindamycin hydrochloride	1903009-01	31
Euro OTC	Clindamycin hydrochloride	200104401	1
Euro OTC	Clindamycin hydrochloride	2001044-01	21
Euro OTC	Clindamycin hydrochloride	200400101	2
Euro OTC	Clindamycin hydrochloride	2004001-01	18
Euro OTC	Clindamycin hydrochloride	2004001-02	1
Euro OTC	Clindamycin hydrochloride	2004001-03	1
Euro OTC	Clindamycin hydrochloride	2201043-01	13
Euro OTC	Clindamycin hydrochloride	220801-01	2
Euro OTC	Clindamycin hydrochloride	2208011-01	4
Euro OTC	Clindamycin hydrochloride	230703101	1
Euro OTC	Clindamycin hydrochloride	25071401	1
Euro OTC	Clindamycin hydrochloride	2908019-01	1
Euro OTC	Clindamycin hydrochloride	2908019V-03	4
Euro OTC	Clindamycin hydrochloride	4988149	1
Euro OTC	Clindamycin hydrochloride	700168	1
Euro OTC	Clindamycin hydrochloride	8061801	1
Euro OTC	Clindamycin hydrochloride	813M-03534	1
Euro OTC	Clindamycin hydrochloride	P-301-CN20181044	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Clindamycin hydrochloride	P-301-CN20210601	1
Euro OTC	Clindamycin hydrochloride	SCHE1107035	1
Euro OTC	Clindamycin hydrochloride	T03-05/1401041-01	1
Euro/Gehe16.03.16	Clindamycin hydrochloride	1510038-01	1
Europharm/Otto	Clindamycin hydrochloride	1111058-01	1
Fagron	Clindamycin hydrochloride	1010616	1
Fagron	Clindamycin hydrochloride	111105803	1
Fagron	Clindamycin hydrochloride	12C19-N06	1
Fagron	Clindamycin hydrochloride	12F19-N07	3
Fagron	Clindamycin hydrochloride	1370983	1
Fagron	Clindamycin hydrochloride	13A22/N01	1
Fagron	Clindamycin hydrochloride	13A22-N01	6
Fagron	Clindamycin hydrochloride	13C15-N06	1
Fagron	Clindamycin hydrochloride	13G24N09	1
Fagron	Clindamycin hydrochloride	13G24-N09	7
Fagron	Clindamycin hydrochloride	13J03-B02	1
Fagron	Clindamycin hydrochloride	13J03-B02_288654	1
Fagron	Clindamycin hydrochloride	13j03-B02-288653	1
Fagron	Clindamycin hydrochloride	13J03B02288654	1
Fagron	Clindamycin hydrochloride	13J03-B02-288654	3
Fagron	Clindamycin hydrochloride	13J03-B02-288655	1
Fagron	Clindamycin hydrochloride	14D23-B03	1
Fagron	Clindamycin hydrochloride	14K04-B05-304995	1
Fagron	Clindamycin hydrochloride	14K04-B05-304996	1
Fagron	Clindamycin hydrochloride	14K04-B05-309851	1
Fagron	Clindamycin hydrochloride	14K04-B05-313090	1
Fagron	Clindamycin hydrochloride	15E06-B12-310472	1
Fagron	Clindamycin hydrochloride	15E06-B12-311886	4
Fagron	Clindamycin hydrochloride	15E06-B12-313089	2
Fagron	Clindamycin hydrochloride	15E06-B12-314064	2
Fagron	Clindamycin hydrochloride	15E06-B12-314065	2
Fagron	Clindamycin hydrochloride	15E06-B12-314066	1
Fagron	Clindamycin hydrochloride	15L22-B03-316670	1
Fagron	Clindamycin hydrochloride	15L22-B03-318787	2
Fagron	Clindamycin hydrochloride	1600324C	1
Fagron	Clindamycin hydrochloride	160324C	2
Fagron	Clindamycin hydrochloride	16D05-B08	4
Fagron	Clindamycin hydrochloride	16D05-B08-320327	3
Fagron	Clindamycin hydrochloride	16D05-B08-321572	1
Fagron	Clindamycin hydrochloride	16D05-B08-323320	1
Fagron	Clindamycin hydrochloride	16D05-B08-323321	1
Fagron	Clindamycin hydrochloride	16D05-B08-325087	1
Fagron	Clindamycin hydrochloride	16D05-B08-325088	3
Fagron	Clindamycin hydrochloride	16d05-b08-325089	1
Fagron	Clindamycin hydrochloride	16D05B08327127	1
Fagron	Clindamycin hydrochloride	16D05-B08-327127	7
Fagron	Clindamycin hydrochloride	16D05-B08-328259	1
Fagron	Clindamycin hydrochloride	16D05-B08-328260	1
Fagron	Clindamycin hydrochloride	16D05-B08-330624	1
Fagron	Clindamycin hydrochloride	16D05-B08-332105	2
Fagron	Clindamycin hydrochloride	16D05-B08-332106	5
Fagron	Clindamycin hydrochloride	16d05-b08-332107	1
Fagron	Clindamycin hydrochloride	16D05-B08-332107	1
Fagron	Clindamycin hydrochloride	16H03-B02	5
Fagron	Clindamycin hydrochloride	16H03-B02-334344	2
Fagron	Clindamycin hydrochloride	16H03-B02-334345	1
Fagron	Clindamycin hydrochloride	16H03-B02-334974	1
Fagron	Clindamycin hydrochloride	16H03-B02-336706	5
Fagron	Clindamycin hydrochloride	16H03-B02-338802	2
Fagron	Clindamycin hydrochloride	16H03-B02-338803	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clindamycin hydrochloride	16H03-B02-339275	1
Fagron	Clindamycin hydrochloride	16H03-B02-341602	2
Fagron	Clindamycin hydrochloride	16-H03-B02-341602	1
Fagron	Clindamycin hydrochloride	16H03-B02-39275	1
Fagron	Clindamycin hydrochloride	16HO3-B02-341602	1
Fagron	Clindamycin hydrochloride	17F22-B07-341603	1
Fagron	Clindamycin hydrochloride	18/15-B04-358084	2
Fagron	Clindamycin hydrochloride	18/15-B04-360142	1
Fagron	Clindamycin hydrochloride	18041801	1
Fagron	Clindamycin hydrochloride	1815B04355580	1
Fagron	Clindamycin hydrochloride	18A18-B08	4
Fagron	Clindamycin hydrochloride	18A18-B08-346106	1
Fagron	Clindamycin hydrochloride	18A18-B08-346107	2
Fagron	Clindamycin hydrochloride	18A18-B08-347483	7
Fagron	Clindamycin hydrochloride	18D11B01	1
Fagron	Clindamycin hydrochloride	18D11-B01	6
Fagron	Clindamycin hydrochloride	18D11-B01-349677	3
Fagron	Clindamycin hydrochloride	18D11-B01-351175	3
Fagron	Clindamycin hydrochloride	18D11-B01-351176	4
Fagron	Clindamycin hydrochloride	18D11-B01-351866	3
Fagron	Clindamycin hydrochloride	18D11-B01-352131	2
Fagron	Clindamycin hydrochloride	18D11-B01-352732	2
Fagron	Clindamycin hydrochloride	18D11-B01-352733	2
Fagron	Clindamycin hydrochloride	18D11-B01-353162	1
Fagron	Clindamycin hydrochloride	18J15-B04	4
Fagron	Clindamycin hydrochloride	18J15-B04-355579	4
Fagron	Clindamycin hydrochloride	18J15-B04-355580	1
Fagron	Clindamycin hydrochloride	18J15-b04-358082	1
Fagron	Clindamycin hydrochloride	18J15-B04-358082	1
Fagron	Clindamycin hydrochloride	18J15-B04-358084	1
Fagron	Clindamycin hydrochloride	18j15-b04-360142	1
Fagron	Clindamycin hydrochloride	18J15-B04-360142	8
Fagron	Clindamycin hydrochloride	18j15b04360143	1
Fagron	Clindamycin hydrochloride	19E23-B02-362301	1
Fagron	Clindamycin hydrochloride	19H28-F06	5
Fagron	Clindamycin hydrochloride	19H28-F06-364300	6
Fagron	Clindamycin hydrochloride	19H28-F06-3643000	1
Fagron	Clindamycin hydrochloride	19H28-F06-3643000855646	1
Fagron	Clindamycin hydrochloride	19H28-F06-364301	10
Fagron	Clindamycin hydrochloride	19H28-F06-364302	8
Fagron	Clindamycin hydrochloride	19H28-F06-366145	6
Fagron	Clindamycin hydrochloride	19H28-F06-366146	7
Fagron	Clindamycin hydrochloride	19H28-F06-366147	5
Fagron	Clindamycin hydrochloride	19H28-F06-366854	1
Fagron	Clindamycin hydrochloride	19H8-F06364302	1
Fagron	Clindamycin hydrochloride	20A27-F01	3
Fagron	Clindamycin hydrochloride	20A27-F01_369463	1
Fagron	Clindamycin hydrochloride	20A27-F01-3694602	1
Fagron	Clindamycin hydrochloride	20A27-F01-369462	2
Fagron	Clindamycin hydrochloride	20A27-F01-369463	7
Fagron	Clindamycin hydrochloride	20D07-F01	3
Fagron	Clindamycin hydrochloride	20D07-F01-370643	2
Fagron	Clindamycin hydrochloride	20D07-F01-370644	1
Fagron	Clindamycin hydrochloride	20D07-F01-370645	5
Fagron	Clindamycin hydrochloride	20D07-F01-370646	1
Fagron	Clindamycin hydrochloride	20D07F01-3709803	1
Fagron	Clindamycin hydrochloride	20D07-F01-370983	3
Fagron	Clindamycin hydrochloride	20H18-F02-374182	3
Fagron	Clindamycin hydrochloride	20J02F03376986	1
Fagron	Clindamycin hydrochloride	21D09-F01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clindamycin hydrochloride	21D09-F01-3784605	1
Fagron	Clindamycin hydrochloride	21D09-F01-378464	1
Fagron	Clindamycin hydrochloride	21D09-F01-378465	6
Fagron	Clindamycin hydrochloride	21D09-F01-378495	1
Fagron	Clindamycin hydrochloride	21G01-F01	2
Fagron	Clindamycin hydrochloride	21G01-F01-379129	6
Fagron	Clindamycin hydrochloride	21G01-F01-379598	6
Fagron	Clindamycin hydrochloride	21G01F01379599	1
Fagron	Clindamycin hydrochloride	21G01-F01379599	1
Fagron	Clindamycin hydrochloride	21G01-F01-379599	12
Fagron	Clindamycin hydrochloride	21G01-F01-379600	10
Fagron	Clindamycin hydrochloride	2208011-01	1
Fagron	Clindamycin hydrochloride	22A31-F04-381645	2
Fagron	Clindamycin hydrochloride	22A31-F04-381646	2
Fagron	Clindamycin hydrochloride	22A31-F04-382349	1
Fagron	Clindamycin hydrochloride	22A31-F04-382350	2
Fagron	Clindamycin hydrochloride	22A31-F04-382351	3
Fagron	Clindamycin hydrochloride	22A31-F04-383139	2
Fagron	Clindamycin hydrochloride	2714Q-03534	1
Fagron	Clindamycin hydrochloride	2816	1
Fagron	Clindamycin hydrochloride	700168-0001	1
Fagron	Clindamycin hydrochloride	700168-0004	1
Fagron	Clindamycin hydrochloride	700168-0009	1
Fagron	Clindamycin hydrochloride	700168-F01-379600	1
Fagron	Clindamycin hydrochloride	B04-3580803	1
Fagron	Clindamycin hydrochloride	F01-3706404	1
Fagron	Clindamycin hydrochloride	F01-3706405	2
Fagron	Clindamycin hydrochloride	F01-370645	1
Fagron	Clindamycin hydrochloride	F01-3791209	1
Fagron	Clindamycin hydrochloride	F02-3741802	2
Fagron	Clindamycin hydrochloride	F03-3769806	1
Fagron	Clindamycin hydrochloride	F06-3643000	1
Fagron	Clindamycin hydrochloride	F06-3643002	1
Fagron	Clindamycin hydrochloride	F06-3661405	1
Fagron	Clindamycin hydrochloride	Fagron20H18-F02-374182	1
Fagron	Clindamycin hydrochloride	K-171217B	2
Fagron	Clindamycin hydrochloride	K-171219B	2
Fagron	Clindamycin hydrochloride	K-180507B	8
Fagron	Clindamycin hydrochloride	K-190507B	1
Fagron	Clindamycin hydrochloride	K-190610B	7
Fagron	Clindamycin hydrochloride	K-190909B	1
Fagron	Clindamycin hydrochloride	K-191226B	1
Fagron	Clindamycin hydrochloride	K-200516B	1
Fagron	Clindamycin hydrochloride	k-210407B	1
Fagron	Clindamycin hydrochloride	K-210407B	4
Fagron	Clindamycin hydrochloride	P-003-CN20150406	1
Fagron	Clindamycin hydrochloride	P003-WS10100301	1
Fagron	Clindamycin hydrochloride	P003WS13091401	1
Fagrun	Clindamycin hydrochloride	18A18-B08-346107	1
Fargon/Noweda	Clindamycin hydrochloride	18D11-B01	1
Fargon/Sanacorp	Clindamycin hydrochloride	K-180507B	1
Fargon	Clindamycin hydrochloride	11L20-No5	1
Fargon	Clindamycin hydrochloride	16D05-B08-320327	1
Fargron/Noweda	Clindamycin hydrochloride	18J15-B04-358084	1
Fargron/Noweda	Clindamycin hydrochloride	19H28-F06-364302	3
Fiebig	Clindamycin hydrochloride	11023741802	1
Fiebig	Clindamycin hydrochloride	f01-3706405	1
Fiebig	Clindamycin hydrochloride	F06-3643002	1
Fiebig	Clindamycin hydrochloride	K-190909B	1
Gehe/ Euro	Clindamycin hydrochloride	1903009-01	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe/EuRho	Clindamycin hydrochloride	2004001-01	1
Gehe/EuRho	Clindamycin hydrochloride	2208011-01	1
Gehe	Clindamycin hydrochloride	11E12-N02	1
Gehe	Clindamycin hydrochloride	11K04-N12	1
Gehe	Clindamycin hydrochloride	13a22-n01	1
Gehe	Clindamycin hydrochloride	13A22-N01	1
GEHE	Clindamycin hydrochloride	1811003-01	1
Gehe	Clindamycin hydrochloride	19H28-F06	1
Gehe	Clindamycin hydrochloride	20A27-F01-369462	1
Gehe	Clindamycin hydrochloride	22G06-F01-383866	1
Gehe	Clindamycin hydrochloride	22G06-F01-383867	1
Gehe	Clindamycin hydrochloride	700168-0002	1
Gehe	Clindamycin hydrochloride	K-210407B	1
gfsdgs	Clindamycin hydrochloride	sgfsgf	1
GUMO	Clindamycin hydrochloride	21000113010	1
hfdhsdhsh	Clindamycin hydrochloride	dfhdhsd	1
Jenne	Clindamycin hydrochloride	18D11-B01-352732	2
Jenne	Clindamycin hydrochloride	18J15-B04-360142	1
L12	Clindamycin hydrochloride	17209302	1
L12	Clindamycin hydrochloride	18009402	2
L12	Clindamycin hydrochloride	18009403	2
L30	Clindamycin hydrochloride	17209301	1
Noweda/EuRho	Clindamycin hydrochloride	2201043-01	1
noweda	Clindamycin hydrochloride	1511004-03	1
Noweda	Clindamycin hydrochloride	1811003-01	1
Noweda	Clindamycin hydrochloride	18D11-B01-351176	1
Noweda	Clindamycin hydrochloride	22001232002	1
Noweda	Clindamycin hydrochloride	22001232003	2
Noweda	Clindamycin hydrochloride	22G06-F01	1
Noweda	Clindamycin hydrochloride	22G06-F01-383867	1
Noweda	Clindamycin hydrochloride	2908019V-03	1
Otto Geilenkirchen	Clindamycin hydrochloride	200400101	1
Phoenix 5.12.2018	Clindamycin hydrochloride	18A18-B08-346106	1
Phoenix	Clindamycin hydrochloride	16D05-B08-327127	1
Phoenix	Clindamycin hydrochloride	1710013-010	1
Phoenix	Clindamycin hydrochloride	1811003-01	1
Phoenix	Clindamycin hydrochloride	2004001-01	1
Phoenix	Clindamycin hydrochloride	3367	1
Phoenix	Clindamycin hydrochloride	K-171217B	1
Phönix	Clindamycin hydrochloride	12H30-N04	1
Phönix	Clindamycin hydrochloride	15392803	1
phönix	Clindamycin hydrochloride	15392820	1
Phönix	Clindamycin hydrochloride	193087005	1
Phönix	Clindamycin hydrochloride	2001044-01	1
Phönix	Clindamycin hydrochloride	20D07-F011	1
rfgrgrgr	Clindamycin hydrochloride		1
Sanacorp	Clindamycin hydrochloride	1511004-03	1
Sanacorp	Clindamycin hydrochloride	16D05-B08-332106	1
Sanacorp	Clindamycin hydrochloride	16H03-B02-339275	1
Sanacorp	Clindamycin hydrochloride	16H03-B02-341602	1
Sanacorp	Clindamycin hydrochloride	18A18-B08-347483	1
Sanacorp	Clindamycin hydrochloride	18D11-B01-352732	1
Sanacorp	Clindamycin hydrochloride	21462-39-S	1
Sanacorp	Clindamycin hydrochloride	21G01-F01-379600	1
Sanacorp	Clindamycin hydrochloride	220801-01	1
Sanacorp	Clindamycin hydrochloride	2208011-01	1
Sanacorp	Clindamycin hydrochloride	22G06-F01-384360	2
Sanacorp	Clindamycin hydrochloride	F01-3694602	1
Sanacorp	Clindamycin hydrochloride	K-171219B	1
Sanacorp	Clindamycin hydrochloride	K-180507B	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Spangro 22.05.2014	Clindamycin hydrochloride	13G24-N09	1
Spangro_04.04.2019	Clindamycin hydrochloride	18D11-B01-352131	1

- 234 982 spectra from 1515 *Apo-Ident* customers from a total of 48 925 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Clindamycin hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Clindamycin hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	640	0	152 322
Type B	0	790	0	201 294
Type C	0	1078	7	234 982

The substance/substance group *Clindamycin hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0625 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2405 %)
Type C	100.0000 % (> 99.9007 %)	99.3548 % (> 99.0783 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20757	21996	8.10	70.47
21224	21224	0.00	71.79
21996	21996	0.00	70.72
22224	22224	0.00	69.82

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22958	22224	9.12	71.11
23245	22224	3.74	70.19
23264	21996	3.44	70.07
25074	25074	0.00	69.59
25307	25307	0.00	71.97
25927	21996	13.84	69.65
27423	21996	18.82	72.68

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Clindamycin-2-dihydrogen phosphate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10003687-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Clindamycin-2-dihydrogen phosphate; Clindamycini phosphas

Special notes

When selecting the *Clindamycin-2-dihydrogen phosphate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Clindamycin-2-dihydrogen phosphate	10	3	8

Second-stage model

For differentiation of the substance/substance group *Clindamycin-2-dihydrogen phosphate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Clindamycin-2-dihydrogen phosphate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	66.87	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Clindamycin-2-dihydrogen phosphate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Clindamycin-2-dihydrogen phosphate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Clindamycin-2-dihydrogen …	13166605	21063	40	1403485
Caelo	Clindamycin-2-dihydrogen …	13166605	21116	40	20130624
Caelo	Clindamycin-2-dihydrogen …	14257305	21798	60	AR-15-FG-015412-01
Caelo	Clindamycin-2-dihydrogen …	15435801	22312	60	AR-16-FG-009129-01
Caelo	Clindamycin-2-dihydrogen …	163265	23055	40	20161214*
Caelo	Clindamycin-2-dihydrogen …	16326504	23586	40	AR-17-FG-022557-01
Caelo	Clindamycin-2-dihydrogen …	20002497001	25389	40	20200922
Caelo	Clindamycin-2-dihydrogen …	21003094	25849	50	20211007*
Caelo	Clindamycin-2-dihydrogen …	22000385	26022	40	20220317*
Caelo	Clindamycin-2-dihydrogen …	22001647	26246	40	20220622*
Caelo	Clindamycin-2-dihydrogen …	22001647	26246SI	20	20220622*
Caelo	Clindamycin-2-dihydrogen …	24000953	27242	40	20240529*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 510 spectra of 12 reference samples from the substance/substance group *Clindamycin-2-dihydrogen phosphate*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 452 spectra from a total of 2832 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 5 reference samples from the substance/substance group *Clindamycin-2-dihydrogen phosphate*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Clindamycin-2-dihydrogen …	172964	24047	40
Caelo	Clindamycin-2-dihydrogen …	191224	24729	40
Caelo	Clindamycin-2-dihydrogen …	23001027	26846	40
Caelo	Clindamycin-2-dihydrogen …	22000385	26022SI†	10
Caelo	Clindamycin-2-dihydrogen …	23001027	26846SI	20

- 201 934 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 18 spectra from 11 *Apo-Ident* customers from 9 batches from the substance/substance group *Clindamycin-2-dihydrogen phosphate*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Clindamycin-2-dihydrogen …	23001027002	1
Caelo	Clindamycin-2-dihydrogen …	14257305	1
Caelo	Clindamycin-2-dihydrogen …	16326507	1
Caelo	Clindamycin-2-dihydrogen …	17344101	6
Caelo	Clindamycin-2-dihydrogen …	17344102	1
Caelo	Clindamycin-2-dihydrogen …	19122402	3
Caelo	Clindamycin-2-dihydrogen …	22000385002	1
Caesar & Loretz GmbH	Clindamycin-2-dihydrogen …	19122401	1
Caesar & Loretz GmbH	Clindamycin-2-dihydrogen …	19122402	2
Noweda	Clindamycin-2-dihydrogen …	23001027001	1

- 236 049 spectra from 1515 *Apo-Ident* customers from a total of 49 249 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Clindamycin-2-dihydrogen phosphate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Clindamycin-2-dihydrogen phosphate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	510	0	152 452
Type B	0	150	0	201 934
Type C	0	18	0	236 049

The substance/substance group *Clindamycin-2-dihydrogen phosphate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8235 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21063	21063	0.00	117.13
21116	21063	2.97	117.06
21798	21798	0.00	118.60
22312	22312	0.00	120.42
23055	23055	0.00	133.13
23586	23586	0.00	142.35
25389	23586	64.84	129.41
25849	25849	0.00	134.65
26022	26022	0.00	149.95
26246	26246	0.00	145.83
27242	27242	0.00	100.63

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Clioquinol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20095-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Clioquinol; Clioquinolum

Special notes

When selecting the *Clioquinol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Clioquinol	7	13	344

Second-stage model

For differentiation of the substance/substance group *Clioquinol* the following second-stage model is used:

- Submodel 12

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Clioquinol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Dithranol	114.58	–
⋮	⋮	⋮
Mesalazine	>50	25.56
Miconazole nitrate	>50	41.94
Theophylline-ethylenediamine hydrate	>50	60.48
Nicotinic acid	>50	76.82

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Clioquinol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Clioquinol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Clioquinol	11304120	20895	40	20111208
Caelo	Clioquinol	163072	23047	40	20161202*
Euro OTC	Clioquinol	1309009-02	21246	40	AR-15-FG-009542-01
Euro OTC	Clioquinol	1509038	21944	60	20151009*
Euro OTC	Clioquinol	2309015	27002	40	20231120*
Fagron	Clioquinol	13I26-N15	21236	40	20131028
Fagron	Clioquinol	14I11-B03-300049	21913	60	20140926
Fagron	Clioquinol	14I11-B03-300049	21972	60	20140926

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 380 spectra of 8 reference samples from the substance/substance group *Clioquinol*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 582 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 570 spectra of 16 reference samples from the substance/substance group *Clioquinol*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Clioquinol	13114413	21308	40
Caelo	Clioquinol	16307206	22960	40
Caelo	Clioquinol	172046	23633	40
Caelo	Clioquinol	182782	24374	40
Caelo	Clioquinol	21000089	25923	40
Caelo	Clioquinol	22000908001	26413	40
Caelo	Clioquinol	23000424	26850	40
Euro OTC	Clioquinol	1612020	22985	40
Euro OTC	Clioquinol	1903010	24624	40
Euro OTC	Clioquinol	1910030	24968	40
Euro OTC	Clioquinol	2011013	25566	40
Euro OTC	Clioquinol	2208002	26268	40
Fagron	Clioquinol	21J01-B08-218979	26159	40
Caelo	Clioquinol	21000089	25923SI	10
Euro OTC	Clioquinol	2208002	26268SI	20
Fagron	Clioquinol	21J01-B08-218979	26159SI	20

- 201 514 spectra from a total of 4032 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1991 spectra from 825 *Apo-Ident* customers from 356 batches from the substance/substance group *Clioquinol*.
- Among them are spectra of independent samples from 344 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Clioquinol	22000908001	1
	Clioquinol	22000908003	2
	Clioquinol	22000908007	2
	Clioquinol	22000908008	3
	Clioquinol	22000908011	1
	Clioquinol	22000908012	10
	Clioquinol	220009098008	1
	Clioquinol	22001088008	1
	Clioquinol	2208002-01	6
	Clioquinol	2208002-02	2
	Clioquinol	22G25-B03-227776	2
	Clioquinol	22G25-B03-2278803	1
	Clioquinol	23000424001	20
	Clioquinol	23000424003	1
	Clioquinol	23000424004	1
	Clioquinol	23000424007	4
	Clioquinol	23003409006	3
	Clioquinol	2300424001	1
	Clioquinol	2300424003	1
	Clioquinol	8069D22	2
	Clioquinol	B03-2277706	1
aelo/Noweda	Clioquinol	21000089001	1
AHD	Clioquinol	1612020-01	1
AHD	Clioquinol	18011502	1
AHD	Clioquinol	2011013-01	1
AHD	Clioquinol	2208002	1
Alliance Healthcare	Clioquinol	19120-B01-196485	1
Alliance Healthcare	Clioquinol	22000908001	1
Alliance	Clioquinol	182782002	1
Alliance	Clioquinol	2011013-01	1
Alliance	Clioquinol	22000908001	1
Alliance	Clioquinol	2205002-01	1
Alliance	Clioquinol	23000424001	1
Anzag	Clioquinol	12L04-N08	1
anzag	Clioquinol	13114418	1
Anzag	Clioquinol	18011517	3
Anzag	Clioquinol	18278210	1
Anzag	Clioquinol	22001088008	1
Anzag	Clioquinol	23000424001	3
Anzag	Clioquinol	23000424003	1
Apo-ident	Clioquinol	1509038-02	1
apo-ident	Clioquinol	1612020-02	1
apomix	Clioquinol	1509038-02	1
Axyntis Group	Clioquinol	1301014-02	1
Axyntis Group	Clioquinol	1301014-03	1
Axyntis Group	Clioquinol	1612020-02	1
Axyntis Group	Clioquinol	F001461	1
Bombastus	Clioquinol	14359118	1
Bombastus	Clioquinol	1509038-03	1
Bombastus	Clioquinol	1903010-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Cael Sanacorp 05.02.2016	Clioquinol	14359103	1
Caelo	Clioquinol	103415	2
Caelo	Clioquinol	10341510	1
Caelo	Clioquinol	10341601	2
Caelo	Clioquinol	10341605	4
Caelo	Clioquinol	10341608	1
Caelo	Clioquinol	11(18011523)	1
Caelo	Clioquinol	1130312	1
Caelo	Clioquinol	11304102	7
Caelo	Clioquinol	11304103	2
Caelo	Clioquinol	11304105	3
Caelo	Clioquinol	11304107	5
Caelo	Clioquinol	11304109	1
Caelo	Clioquinol	11304111	2
Caelo	Clioquinol	11304112	6
Caelo	Clioquinol	11304113	4
Caelo	Clioquinol	11304116	3
Caelo	Clioquinol	11304117	10
Caelo	Clioquinol	11304119	3
Caelo	Clioquinol	11304120	12
Caelo	Clioquinol	11304124	13
Caelo	Clioquinol	1201034-01	1
Caelo	Clioquinol	1201034-02	2
Caelo	Clioquinol	1214I02562	1
Caelo	Clioquinol	12F20-N05	1
Caelo	Clioquinol	12L04-N08	2
Caelo	Clioquinol	130114-02	1
Caelo	Clioquinol	1309009-02	1
Caelo	Clioquinol	13114404	2
Caelo	Clioquinol	13114406	1
Caelo	Clioquinol	13114408	3
Caelo	Clioquinol	13114410	2
Caelo	Clioquinol	13114413	11
Caelo	Clioquinol	13114415	3
Caelo	Clioquinol	13114417	7
Caelo	Clioquinol	13114418	5
Caelo	Clioquinol	13114421	1
Caelo	Clioquinol	13114422	7
Caelo	Clioquinol	13114423	10
Caelo	Clioquinol	13114424	10
Caelo	Clioquinol	13114427	2
Caelo	Clioquinol	13A29-N07	1
Caelo	Clioquinol	14/11-B03-309181	1
Caelo	Clioquinol	14/11-BG03-309181	1
Caelo	Clioquinol	14/-B03-309181	1
Caelo	Clioquinol	1405080031	1
Caelo	Clioquinol	1405080036	1
Caelo	Clioquinol	1409031-01	1
Caelo	Clioquinol	14353120	1
Caelo	Clioquinol	14359102	12
Caelo	Clioquinol	14359103	11
Caelo	Clioquinol	14359111	14
Caelo	Clioquinol	14359112	14
Caelo	Clioquinol	14359113	2
Caelo	Clioquinol	14359116	1
Caelo	Clioquinol	14359117	4
Caelo	Clioquinol	14359118	10
Caelo	Clioquinol	14359119	4
Caelo	Clioquinol	14359120	8
Caelo	Clioquinol	1435918	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clioquinol	144359111	1
Caelo	Clioquinol	14C21-B06-293104	1
Caelo	Clioquinol	1509038-01	1
Caelo	Clioquinol	1509038-02	3
Caelo	Clioquinol	150903803	1
Caelo	Clioquinol	1509038-03	4
Caelo	Clioquinol	1509038-OTC-Pharma	1
Caelo	Clioquinol	15L30-B05-314974	1
Caelo	Clioquinol	15L30-B05-321899	2
Caelo	Clioquinol	16021505	1
Caelo	Clioquinol	1605100084	1
Caelo	Clioquinol	160916CL	1
Caelo	Clioquinol	1612020-01	8
Caelo	Clioquinol	1612020-02	1
Caelo	Clioquinol	1612020-03	1
Caelo	Clioquinol	16122020-01	1
Caelo	Clioquinol	163072	1
Caelo	Clioquinol	16307203	3
Caelo	Clioquinol	16307204	1
Caelo	Clioquinol	16307205	14
Caelo	Clioquinol	16307206	23
Caelo	Clioquinol	16307207	23
Caelo	Clioquinol	163072073	1
Caelo	Clioquinol	16307208	17
Caelo	Clioquinol	16307209	1
Caelo	Clioquinol	16307210	6
Caelo	Clioquinol	16307211	9
Caelo	Clioquinol	16307213	1
Caelo	Clioquinol	16307214	18
Caelo	Clioquinol	16307215	15
Caelo	Clioquinol	16307216	18
Caelo	Clioquinol	16I18-B04-332852	1
Caelo	Clioquinol	16J18-B04-328520	1
Caelo	Clioquinol	16l18-B04-329141	1
Caelo	Clioquinol	170926CL/16307208	1
Caelo	Clioquinol	172041603	1
Caelo	Clioquinol	17204601	4
Caelo	Clioquinol	17204603	22
Caelo	Clioquinol	172046303	1
Caelo	Clioquinol	18011501	2
Caelo	Clioquinol	18011502	48
Caelo	Clioquinol	18011511	2
Caelo	Clioquinol	180115117	1
Caelo	Clioquinol	18011516	39
Caelo	Clioquinol	18011516P-190705-1	1
Caelo	Clioquinol	18011517	2
Caelo	Clioquinol	18011523	30
Caelo	Clioquinol	18011527	1
Caelo	Clioquinol	180127C/16307215	1
Caelo	Clioquinol	1801523	1
Caelo	Clioquinol	18121714	1
Caelo	Clioquinol	1827782008	1
Caelo	Clioquinol	18278002	1
Caelo	Clioquinol	182782002	43
Caelo	Clioquinol	182782003	1
Caelo	Clioquinol	182782007	1
Caelo	Clioquinol	182782008	15
Caelo	Clioquinol	182782009	15
Caelo	Clioquinol	18278202	4
Caelo	Clioquinol	18278205	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clioquinol	18278206	22
Caelo	Clioquinol	18278210	9
Caelo	Clioquinol	18278214	29
Caelo	Clioquinol	18278215	24
Caelo	Clioquinol	182792008	1
Caelo	Clioquinol	18E08-B06-355575	2
Caelo	Clioquinol	19I2O-B01-196485	1
Caelo	Clioquinol	20001561001	2
Caelo	Clioquinol	20001561003	6
Caelo	Clioquinol	20001561006	5
Caelo	Clioquinol	2001561001	2
Caelo	Clioquinol	2011013-01	1
Caelo	Clioquinol	21000089001	50
Caelo	Clioquinol	21000089004	5
Caelo	Clioquinol	21000089006	28
Caelo	Clioquinol	2100008901	2
Caelo	Clioquinol	21000089011	21
Caelo	Clioquinol	21000089015	3
Caelo	Clioquinol	210000899004	1
Caelo	Clioquinol	21000098006	1
Caelo	Clioquinol	2100089001	1
Caelo	Clioquinol	22000308003	1
Caelo	Clioquinol	220009080001	1
Caelo	Clioquinol	220009080003	1
Caelo	Clioquinol	22000908001	19
Caelo	Clioquinol	22000908003	4
Caelo	Clioquinol	22000908008	6
Caelo	Clioquinol	22000908011	1
Caelo	Clioquinol	22000908012	1
Caelo	Clioquinol	22001088003	10
Caelo	Clioquinol	22001088004	1
Caelo	Clioquinol	23000424001	1
Caelo	Clioquinol	2773	1
Caelo	Clioquinol	3041409	1
Caelo	Clioquinol	3513I-02562	1
Caelo	Clioquinol	3713A2562	1
Caelo	Clioquinol	4111707	1
Caelo	Clioquinol	4214Q-02562	1
Caelo	Clioquinol	4613E2562	1
Caelo	Clioquinol	5031302	1
Caelo	Clioquinol	5089	1
Caelo	Clioquinol	5213A2562	1
Caelo	Clioquinol	8714	1
Caelo	Clioquinol	B01-1964805	1
Caesar & Lorenz GmbH	Clioquinol	14359112	1
Caesar & Loretz GmbH...	Clioquinol	21000089004	1
Caesar & Loretz GmbH...	Clioquinol	21000089001	1
Caesar & Loretz GmbH...	Clioquinol	21000089006	1
Caesar & Loretz GmbH...	Clioquinol	22001088003	1
Caesar & Loretz GmbH...	Clioquinol	18278214	2
Caesar & Loretz GmbH...	Clioquinol	18278215	1
Caesar & Loretz GmbH...	Clioquinol	21000089001	3
Caesar & Loretz GmbH...	Clioquinol	21000089001	1
Caesar & Loretz GmbH/AEP	Clioquinol	21000089012	1
Caesar & Loretz GmbH/AHD	Clioquinol	18011523	1
Caesar & Loretz GmbH/AHD	Clioquinol	22000908008	1
Caesar & Loretz GmbH/AHD	Clioquinol	22001088003	1
Caesar & Loretz GmbH/Alli	Clioquinol	18278215	1
Caesar & Loretz GmbH...	Clioquinol	21000089001	1
Caesar & Loretz GmbH...	Clioquinol	18011502	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Clioquinol	21000089001	1
Caesar & Loretz GmbH/Gehe	Clioquinol	182782002	1
Caesar & Loretz GmbH/Gehe	Clioquinol	21000089006	1
Caesar & Loretz GmbH/Gehe	Clioquinol	22001088004	2
Caesar & Loretz GmbH...	Clioquinol	22000908003	1
Caesar & Loretz GmbH...	Clioquinol	21000089001	1
Caesar & Loretz GmbH...	Clioquinol	21000089001	1
Caesar & Loretz GmbH...	Clioquinol	21000089001	1
Caesar & Loretz GmbH...	Clioquinol	21000089004	1
Caesar & Loretz GmbH...	Clioquinol	22001088008	1
Caesar & Loretz GmbH/K	Clioquinol	182782009	1
Caesar & Loretz GmbH/Kehr	Clioquinol	182782008	1
Caesar & Loretz GmbH...	Clioquinol	18278202	1
Caesar & Loretz GmbH/Ph	Clioquinol	18278214	1
Caesar & Loretz GmbH...	Clioquinol	20001561006	1
Caesar & Loretz GmbH...	Clioquinol	22000908001	1
Caesar & Loretz GmbH...	Clioquinol	182782008	1
Caesar & Loretz GmbH...	Clioquinol	21000089001	1
Caesar & Loretz GmbH...	Clioquinol	21000089015	1
Caesar & Loretz GmbH...	Clioquinol	22000908008	2
Caesar & Loretz GmbH...	Clioquinol	182782008	1
Caesar & Loretz GmbH...	Clioquinol	182782009	1
Caesar & Loretz GmbH...	Clioquinol	18278214	1
Caesar & Loretz GmbH...	Clioquinol	20001561006	1
Caesar & Loretz GmbH...	Clioquinol	21000089011	1
Caesar & Loretz GmbH...	Clioquinol	22001088004	1
Caesar & Loretz GmbH	Clioquinol	1612020-02	1
Caesar & Loretz GmbH	Clioquinol	16307207	1
Caesar & Loretz GmbH	Clioquinol	16307216	1
Caesar & Loretz GmbH	Clioquinol	18011516	5
Caesar & Loretz GmbH	Clioquinol	18011517	3
Caesar & Loretz GmbH	Clioquinol	18011523	3
Caesar & Loretz GmbH	Clioquinol	18273214	1
Caesar & Loretz GmbH	Clioquinol	182778215	1
Caesar & Loretz GmbH	Clioquinol	182782002	10
Caesar & Loretz GmbH	Clioquinol	182782003	1
Caesar & Loretz GmbH	Clioquinol	182782006	1
Caesar & Loretz GmbH	Clioquinol	182782008	5
Caesar & Loretz GmbH	Clioquinol	182782009	3
Caesar & Loretz GmbH	Clioquinol	18278202	1
Caesar & Loretz GmbH	Clioquinol	18278206	2
Caesar & Loretz GmbH	Clioquinol	18278210	2
Caesar & Loretz GmbH	Clioquinol	18278214	11
Caesar & Loretz GmbH	Clioquinol	18278215	5
Caesar & Loretz GmbH	Clioquinol	20001561003	1
Caesar & Loretz GmbH	Clioquinol	20001561006	2
Caesar & Loretz GmbH	Clioquinol	21000089001	11
Caesar & Loretz GmbH	Clioquinol	21000089004	2
Caesar & Loretz GmbH	Clioquinol	21000089006	12
Caesar & Loretz GmbH	Clioquinol	21000089011	2
Caesar & Loretz GmbH	Clioquinol	21000089012	2
Caesar & Loretz GmbH	Clioquinol	21000089015	2
Caesar & Loretz GmbH	Clioquinol	22000908001	8
Caesar & Loretz GmbH	Clioquinol	22000908003	2
Caesar & Loretz GmbH	Clioquinol	22001088003	5
Caesar & Loretz GmbH	Clioquinol	22001088004	2
Caesar & Loretz GmbH	Clioquinol	23000424001	2
Caesar & Loretz Hilden	Clioquinol	18011516	1
Caesar & Loretz Hilden	Clioquinol	18011523	1
Caesar & Loretz/Noweda	Clioquinol	182782008	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz	Clioquinol	18011502	1
Caesar&Lorenz	Clioquinol	2100089001	1
caesar&loretz,Phönix	Clioquinol	14359111	1
Caolo- Noweda	Clioquinol	14359118	1
Cealo/ Anzag	Clioquinol	16307215	1
Cealo/Sanacorp	Clioquinol	1309009-01	1
Cealo/Sanacorp	Clioquinol	18278206	1
Ebert & Jacobi	Clioquinol	14359103	1
EuRho / Gehe	Clioquinol	1910030-01	2
EuRho/Gehe	Clioquinol	1910030-02	2
EuRho/Phönix	Clioquinol	1903010-01	1
Eurho/Phönix	Clioquinol	1910030-01	1
Eurho/Phönix	Clioquinol	201101301	1
EuRho	Clioquinol	1201034-02	1
EuRho	Clioquinol	1309009-02	1
EuRho	Clioquinol	161202001	1
EuRho	Clioquinol	1612020-01	1
EuRho	Clioquinol	1612020-02	1
EuRho	Clioquinol	1910030-02	1
Eurho	Clioquinol	2011013-01	1
EuRho	Clioquinol	201101301	1
EuRho	Clioquinol	2011013-01	3
EURO / Sanacorp	Clioquinol	150903802	1
Euro OTC	Clioquinol		1
Euro OTC	Clioquinol	1102022-01	2
Euro OTC	Clioquinol	1102022-02	3
Euro OTC	Clioquinol	1201034-01	5
Euro OTC	Clioquinol	120103402	1
Euro OTC	Clioquinol	1201034-02	8
Euro OTC	Clioquinol	1213A-02562	1
Euro OTC	Clioquinol	13010104-03	1
Euro OTC	Clioquinol	1301014	1
Euro OTC	Clioquinol	1301014-01	2
Euro OTC	Clioquinol	1301014-02	6
Euro OTC	Clioquinol	1301041-01	1
Euro OTC	Clioquinol	1303009-02	1
Euro OTC	Clioquinol	1305070109	1
Euro OTC	Clioquinol	1309009-01	7
Euro OTC	Clioquinol	130900902	1
Euro OTC	Clioquinol	1309009-02	14
Euro OTC	Clioquinol	1405080031	1
Euro OTC	Clioquinol	14090131-02	1
Euro OTC	Clioquinol	140903101	1
Euro OTC	Clioquinol	1409031-01	5
Euro OTC	Clioquinol	1409031-02	11
Euro OTC	Clioquinol	14359118	1
Euro OTC	Clioquinol	14359120	1
Euro OTC	Clioquinol	150903-01	1
Euro OTC	Clioquinol	1509038	2
Euro OTC	Clioquinol	1509038-0	1
Euro OTC	Clioquinol	1509038-01	13
Euro OTC	Clioquinol	150903802	2
Euro OTC	Clioquinol	1509038-02	40
Euro OTC	Clioquinol	1509038-03	30
Euro OTC	Clioquinol	150903804	1
Euro OTC	Clioquinol	1509038-04	5
Euro OTC	Clioquinol	1509038-31	1
Euro OTC	Clioquinol	1605100084	1
Euro OTC	Clioquinol	1612020	3
Euro OTC	Clioquinol	1612020_01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Clioquinol	161202001	3
Euro OTC	Clioquinol	1612020-01	44
Euro OTC	Clioquinol	1612020-02	20
Euro OTC	Clioquinol	161202003	1
Euro OTC	Clioquinol	1612020-03	26
Euro OTC	Clioquinol	1612022001	1
Euro OTC	Clioquinol	16307208	1
Euro OTC	Clioquinol	16307216	1
Euro OTC	Clioquinol	16J18-B04	1
Euro OTC	Clioquinol	1903010	1
Euro OTC	Clioquinol	1903010-01	10
Euro OTC	Clioquinol	19100030-02	1
Euro OTC	Clioquinol	1910020-01	1
Euro OTC	Clioquinol	1910030	2
Euro OTC	Clioquinol	19100300-01	1
Euro OTC	Clioquinol	191003001	2
Euro OTC	Clioquinol	1910030-01	18
Euro OTC	Clioquinol	191003002	3
Euro OTC	Clioquinol	1910030-02	24
Euro OTC	Clioquinol	2011013-01	30
Euro OTC	Clioquinol	211013-01	1
Euro OTC	Clioquinol	2195137	1
Euro OTC	Clioquinol	22022021-1	1
Euro OTC	Clioquinol	2208002-01	6
Euro OTC	Clioquinol	2507212562	1
Euro OTC	Clioquinol	3719U-02562	1
Euro OTC	Clioquinol	5219E32562	1
Euro OTC	Clioquinol	PC86	1
Euro OTC	Clioquinol	RetestCharge24619/3	1
Euro/Phoenix	Clioquinol	1612020-02	3
Euro/Phönix	Clioquinol	1509038-02	1
Euro	Clioquinol	1509038-01	2
EuRoh	Clioquinol	2011013-01	2
europharm	Clioquinol	1509038	1
Fagron	Clioquinol		1
Fagron	Clioquinol	1005090024	1
Fagron	Clioquinol	11304112	1
Fagron	Clioquinol	11304120	1
Fagron	Clioquinol	11G20/N09	1
Fagron	Clioquinol	11G20-N09	1
Fagron	Clioquinol	11K21-N18	4
Fagron	Clioquinol	1205110014	1
Fagron	Clioquinol	12F20-N05	3
Fagron	Clioquinol	12L04-N08	7
Fagron	Clioquinol	13/26-N15	2
Fagron	Clioquinol	1305120028	1
Fagron	Clioquinol	1309009-01	1
Fagron	Clioquinol	13114417	1
Fagron	Clioquinol	13114423	2
Fagron	Clioquinol	13114424	1
Fagron	Clioquinol	1326-N15	3
Fagron	Clioquinol	13A29-N07	7
Fagron	Clioquinol	13A29-N07-3398310111	1
Fagron	Clioquinol	13D15-N01	8
Fagron	Clioquinol	13DS15-NO1	1
Fagron	Clioquinol	13F12-N20	2
Fagron	Clioquinol	13F12-N200463480	1
Fagron	Clioquinol	13I26N15	1
Fagron	Clioquinol	13I26-N15	5
Fagron	Clioquinol	14/11-803-309181	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clioquinol	14/11-B03-300049	3
Fagron	Clioquinol	14/11-B03-309181	4
Fagron	Clioquinol	14/11-Bo3	1
Fagron	Clioquinol	14052014C	1
Fagron	Clioquinol	1411-813	1
Fagron	Clioquinol	1411B03300049	1
Fagron	Clioquinol	1411-B03-300049	4
Fagron	Clioquinol	1411-B03-309181	1
Fagron	Clioquinol	14359118	1
Fagron	Clioquinol	14C21806293104	1
Fagron	Clioquinol	14C21-B06	2
Fagron	Clioquinol	14c21B06293104	1
Fagron	Clioquinol	14C21B06293104	1
Fagron	Clioquinol	14C21-B06-293104	6
Fagron	Clioquinol	14C21-B06-293132	2
Fagron	Clioquinol	14-C21-B06-293132	1
Fagron	Clioquinol	14C21-B06-297159	3
Fagron	Clioquinol	14C21-B08	1
Fagron	Clioquinol	14I11-B03	2
Fagron	Clioquinol	14I11-B03-3000049	1
Fagron	Clioquinol	14I11B03300049	1
Fagron	Clioquinol	14I11-B03-300049	6
Fagron	Clioquinol	14I11-B03-309048	2
Fagron	Clioquinol	14I11-B03-309181	3
Fagron	Clioquinol	14L11-B03	1
Fagron	Clioquinol	14l11-B03-300049	1
Fagron	Clioquinol	1505120044	1
Fagron	Clioquinol	15L30-321899	1
Fagron	Clioquinol	15L30-B05	2
Fagron	Clioquinol	15L30-B05-314974	8
Fagron	Clioquinol	15L30-B05-319616	2
Fagron	Clioquinol	15L30-B05-321899	7
Fagron	Clioquinol	15L30-B05-321899	1
Fagron	Clioquinol	16/18-b04-328511	1
Fagron	Clioquinol	16/18-B04-328511	1
Fagron	Clioquinol	16/18-B04-332852	2
Fagron	Clioquinol	1605100008	2
Fagron	Clioquinol	1612020-03	1
Fagron	Clioquinol	1618B04-329141	1
Fagron	Clioquinol	16J18B04	1
Fagron	Clioquinol	16J18-B04	2
Fagron	Clioquinol	16J18-B04-328511	8
Fagron	Clioquinol	16J18-B04-328520	2
Fagron	Clioquinol	16J18-B04-32914	1
Fagron	Clioquinol	16j18-b04-329141	1
Fagron	Clioquinol	16j18-B04-329141	1
Fagron	Clioquinol	16J18B04329141	1
Fagron	Clioquinol	16J18-B04-329141	4
Fagron	Clioquinol	16J18-B04-329704	1
Fagron	Clioquinol	16J18-B04-332852	6
Fagron	Clioquinol	16J18-B04-332861	1
Fagron	Clioquinol	17204603	1
Fagron	Clioquinol	18805B07345488	1
Fagron	Clioquinol	18805-B07-3475B6	1
Fagron	Clioquinol	188B05-B07345483	1
Fagron	Clioquinol	18B05-B07	2
Fagron	Clioquinol	18B05-B07-345483	3
Fagron	Clioquinol	18B05-B07-345488	2
Fagron	Clioquinol	18B05-B07-347586	3
Fagron	Clioquinol	18E08-B06	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clioquinol	18E08-B06-350976	2
Fagron	Clioquinol	18E08-B06-352127	4
Fagron	Clioquinol	18E08-B06-355552	2
Fagron	Clioquinol	18E08-B06355575	1
Fagron	Clioquinol	18E08-B06-355575	2
Fagron	Clioquinol	19/20-B01-196485	1
Fagron	Clioquinol	19/20-B01-197294	1
Fagron	Clioquinol	19F17B07-191238	1
Fagron	Clioquinol	19F17-B07-191238	2
Fagron	Clioquinol	19F17-B07-191238/08122I18	1
Fagron	Clioquinol	19F17-B07-191239	3
Fagron	Clioquinol	19I20-B01-196485	4
Fagron	Clioquinol	19I20-B01-1972904	1
Fagron	Clioquinol	19I20-B01-197294	3
Fagron	Clioquinol	19I20-B01-197295	3
Fagron	Clioquinol	19I20-Bo1-196485	1
Fagron	Clioquinol	19l20-B01-196485	1
Fagron	Clioquinol	2011013-01	1
Fagron	Clioquinol	2014Q2562	1
Fagron	Clioquinol	21D01-B08-217230	1
Fagron	Clioquinol	21G22-B05-213512	1
Fagron	Clioquinol	21J01-B08-218979	1
Fagron	Clioquinol	21J01-B08-219069	1
Fagron	Clioquinol	22C15-B07-220931	4
Fagron	Clioquinol	22C15-B07-223056	2
Fagron	Clioquinol	22G25-B03-222915	2
Fagron	Clioquinol	22G25B03227776	1
Fagron	Clioquinol	22G25-B03-227776	1
Fagron	Clioquinol	2514U2562	1
Fagron	Clioquinol	28031401	1
Fagron	Clioquinol	3916U-02562	1
Fagron	Clioquinol	7D20-N03	1
Fagron	Clioquinol	812218	1
Fagron	Clioquinol	8122I18	1
Fagron	Clioquinol	B01-1964805	1
Fagron	Clioquinol	B01-1972904	1
Fargon	Clioquinol	16J18-B04-329704	1
Fiebig	Clioquinol	14/11-B03-300048	1
Fiebig	Clioquinol	1409031-02	2
Fiebig	Clioquinol	19I20-B01-196485	1
Gatt-Koller	Clioquinol	1802295	2
GEHE 04.08.2014	Clioquinol	13114418	1
Gehe amax	Clioquinol	13114418	1
Gehe/EuRho	Clioquinol	1910030-01	1
Gehe	Clioquinol	1409031-02	1
GEHE	Clioquinol	1509038-02	1
Gehe	Clioquinol	1509038-03	1
GEHE	Clioquinol	1509038-03	1
Gehe	Clioquinol	1612020-01	1
Gehe	Clioquinol	16307216	1
Gehe	Clioquinol	18011502	1
GEHE	Clioquinol	18B05-B07	1
Gehe	Clioquinol	22000908004	1
Gehe	Clioquinol	22000908008	1
GEHE	Clioquinol	22000908008	1
Gehe	Clioquinol	22000908012	1
Gehe	Clioquinol	22001088003	1
Gehe	Clioquinol	2208002-01	1
GEHE	Clioquinol	2208002-01	1
Gehe	Clioquinol	2300024003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Clioquinol	23000424007	1
Geibo/EuRho 16.09.2020	Clioquinol	1910030-01	1
Henry Lamote Oils GmbH	Clioquinol	28151-02562	1
Ichthyol-Gesellschaft	Clioquinol	1612020	1
Jenne	Clioquinol	2208002-01	1
Klenk	Clioquinol	11304120	1
L12	Clioquinol	1509038-03	2
L12	Clioquinol	1612020-01	2
M/s Eskayiodine Pvt....	Clioquinol	18278206	1
Nachprüfung	Clioquinol	13L26-N15	2
Nachprüfung	Clioquinol	3021U-02562	1
Nachprüfung	Clioquinol	AP200615-12	1
Noweda/Noweda	Clioquinol	16L18-B04-328520	1
Noweda/Noweda	Clioquinol	16L18-B04-329704	1
Noweda	Clioquinol	10057206	1
Noweda	Clioquinol	11304107	1
Noweda	Clioquinol	11304111	1
Noweda	Clioquinol	1201034-02	2
Noweda	Clioquinol	1309009-01	1
Noweda	Clioquinol	14359103	1
Noweda	Clioquinol	14359120	1
Noweda	Clioquinol	1612020-01	1
Noweda	Clioquinol	16307208	1
Noweda	Clioquinol	17204603	1
Noweda	Clioquinol	18278214	1
Noweda	Clioquinol	18278215	1
Noweda	Clioquinol	1903010-01	1
Noweda	Clioquinol	22000908003	1
Noweda	Clioquinol	22000908012	2
Noweda	Clioquinol	2208002-01	1
Noweda	Clioquinol	22G25-B03-222915	1
Noweda	Clioquinol	22G25-B03-227776	1
Phö/Dr.Wolff	Clioquinol	18011523	1
Phoenix	Clioquinol	11304119	1
Phoenix	Clioquinol	13114408	2
Phoenix	Clioquinol	13114417	1
Phoenix	Clioquinol	1612020-02	1
Phoenix	Clioquinol	16J18-B04-332852	2
Phoenix	Clioquinol	18011523	1
Phoenix	Clioquinol	18278206	1
Phoenix	Clioquinol	21000089001	2
Phoenix	Clioquinol	21000089006	2
Phoenix	Clioquinol	22000908008	1
Phoenix	Clioquinol	22001088003	1
Phoenix	Clioquinol	23000424001	1
Phoenix	Clioquinol	8178L17	1
Phönix Gotha	Clioquinol	11304124	1
phönix	Clioquinol		1
Phönix	Clioquinol	1102022-02	3
Phönix	Clioquinol	1201034-02	1
Phönix	Clioquinol	1309009-02	1
Phönix	Clioquinol	13114417	1
Phönix	Clioquinol	14C21-B06	2
Phönix	Clioquinol	14C21-B08	1
Phönix	Clioquinol	15L30-B05-314974	1
Phönix	Clioquinol	1612020-01	1
Phönix	Clioquinol	16718b04332852	1
Phönix	Clioquinol	182782008	1
Phönix	Clioquinol	1903010-01	1
Phönix	Clioquinol	1910030-02	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Clioquinol	2011013-01	1
Phönix	Clioquinol	21000089001	1
Phönix	Clioquinol	21000089006	1
Phönix	Clioquinol	22000908012	1
Phönix	Clioquinol	3165	1
Sanacorp	Clioquinol	11304111	1
Sanacorp	Clioquinol	11304124	1
Sanacorp	Clioquinol	1201034-01	1
Sanacorp	Clioquinol	13114422	1
Sanacorp	Clioquinol	1612020-03	1
Sanacorp	Clioquinol	16J18-B04-328511	1
Sanacorp	Clioquinol	1910030-01	1
Sanacorp	Clioquinol	20001561006	1
Sanacorp	Clioquinol	22000908004	1
Sanacorp	Clioquinol	22000908007	1
Sanacorp	Clioquinol	22G25-B03-227776	1
Sanacorp	Clioquinol	23000424001	1
Sanacorp	Clioquinol	8/AKD4	1
Sanacorp	Clioquinol	8075E19	1
Sanacorp04	Clioquinol	1612020-02	1
Synthexim / Gehe	Clioquinol	14359118	1
Synthexim	Clioquinol	1405080036	1
Unisan	Clioquinol	14/11-B03	1
VDL	Clioquinol	131144131	1
wepa/Sanaco	Clioquinol	1439118	1

- 234 076 spectra from 1515 *Apo-Ident* customers from a total of 48 907 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Clioquinol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Clioquinol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	570	0	201 514
Type C	0	1986	5	234 076

The substance/substance group *Clioquinol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.9474 %)
Type C	100.0000 % (> 99.9007 %)	99.7489 % (> 99.5982 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20895	23047	6.68	203.70
21236	21246	6.35	202.77
21246	21246	0.00	201.17
21913	21944	6.42	198.87
21944	21944	0.00	198.43
21972	21246	9.46	197.28
23047	23047	0.00	202.38
27002	27002	0.00	179.27

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Clobetasol propionate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20030-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Clobetasol propionate; Clobetasoli propionas

Special notes

When selecting the *Clobetasol propionate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Clobetasol propionate	9	14	593

Second-stage model

For differentiation of the substance/substance group *Clobetasol propionate* the following second-stage model is used:

- Submodel 15

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Clobetasol propionate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Betamethasone dipropionate	52.73	61.97
⋮	⋮	⋮
Beclometasone dipropionate	55.71	64.36

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Clobetasol propionate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Clobetasol propionate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Clobetasol propionate	13134705	21092	80	AR-15-FG-005328-01
Caelo	Clobetasol propionate	13269505	21473	60	AR-15-FG-000622-02
Caelo	Clobetasol propionate	14338001	21802	60	AR-16-FG-008581-01
Caelo	Clobetasol propionate	14338001	21802SI	59	AR-16-FG-008581-01
Caelo	Clobetasol propionate	14338001	21896	59	1607072
Caelo	Clobetasol propionate	14338001	21896SI	45	1607072
Caelo	Clobetasol propionate	15439504	22724	40	20160204
Caelo	Clobetasol propionate	15439504	22724SI	37	20160204
Caelo	Clobetasol propionate	192245	24904	40	20200127*
Euro OTC	Clobetasol propionate	1211021-04	21611	60	1605044
Euro OTC	Clobetasol propionate	1606022	22714	40	20160713*
Euro OTC	Clobetasol propionate	1606022	22714SI	40	20160713*
Euro OTC	Clobetasol propionate	2005025	25349	40	20200917*
Euro OTC	Clobetasol propionate	2005025	25349SI	40	20200917*
Fagron	Clobetasol propionate	18I12-B02-357669	24691	40	20181001

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 740 spectra of 15 reference samples from the substance/substance group *Clobetasol propionate*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 222 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1184 spectra of 30 reference samples from the substance/substance group *Clobetasol propionate*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Clobetasol propionate	161067	22470	60
Caelo	Clobetasol propionate	170967	23665	40
Caelo	Clobetasol propionate	21001700	25793	40
Caelo	Clobetasol propionate	24001314	27311	40
Euro OTC	Clobetasol propionate	1704020	23397	40
Euro OTC	Clobetasol propionate	1804002	24075	40
Euro OTC	Clobetasol propionate	1903014	24615	40
Euro OTC	Clobetasol propionate	2003026	25313	40
Euro OTC	Clobetasol propionate	2109003	25870	50
Euro OTC	Clobetasol propionate	2209014	26428	40
Euro OTC	Clobetasol propionate	2406006	27346	40
Fagron	Clobetasol propionate	19B06-B03-360421	24822	40
Fagron	Clobetasol propionate	22L20-B03-227672	26546	40
Fagron	Clobetasol propionate	23H24-B04-238756	27468	40
Caelo	Clobetasol propionate	161067	22470SI	48
Caelo	Clobetasol propionate	170967	23665SI	20
Caelo	Clobetasol propionate	192245	24904SI†	40
Caelo	Clobetasol propionate	21001700	25793SI	40
Caelo	Clobetasol propionate	24001314	27311SI	34
Euro OTC	Clobetasol propionate	1704020	23397SI	20

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Clobetasol propionate	1804002	24075SI	22
Euro OTC	Clobetasol propionate	1903014	24615SI	40
Euro OTC	Clobetasol propionate	2003026	25313SI	40
Euro OTC	Clobetasol propionate	2109003	25870SI	50
Euro OTC	Clobetasol propionate	2209014	26428SI	40
Euro OTC	Clobetasol propionate	2406006	27346SI	40
Fagron	Clobetasol propionate	18I12-B02-357669	24691SI[†]	40
Fagron	Clobetasol propionate	19B06-B03-360421	24822SI	40
Fagron	Clobetasol propionate	22L20-B03-227672	26546SI	40
Fagron	Clobetasol propionate	23H24-B04-238756	27468SI	40

- 200 900 spectra from a total of 4029 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4444 spectra from 1179 *Apo-Ident* customers from 619 batches from the substance/substance group *Clobetasol propionate*.

- Among them are spectra of independent samples from 592 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Clobetasol propionate	11/29-N07	1
	Clobetasol propionate	18044002-01	1
	Clobetasol propionate	21001700015	1
	Clobetasol propionate	21001700018	1
	Clobetasol propionate	21001700021	3
	Clobetasol propionate	21001700023	5
	Clobetasol propionate	21001700025	6
	Clobetasol propionate	21001700026	3
	Clobetasol propionate	2100170025	1
	Clobetasol propionate	2109003-001	1
	Clobetasol propionate	2109003-01	11
	Clobetasol propionate	21L16-B08-216942	1
	Clobetasol propionate	21L16-B08-221088	1
	Clobetasol propionate	21L16-B08	1
	Clobetasol propionate	22090-01	1
	Clobetasol propionate	2209014_01	1
	Clobetasol propionate	2209014-01	16
	Clobetasol propionate	2209014-02	2
	Clobetasol propionate	22H25-B08-223089	1
	Clobetasol propionate	22H-25-B08-223089	1
	Clobetasol propionate	22H25-B08-223090	1
	Clobetasol propionate	22H25-B08-225386	1
	Clobetasol propionate	22L20-B03-227672	1
	Clobetasol propionate	23000426001	22
	Clobetasol propionate	23000426002	5

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Clobetasol propionate	23000426003	18
	Clobetasol propionate	23000426006	2
	Clobetasol propionate	230033150003	1
	Clobetasol propionate	23003315001	2
	Clobetasol propionate	23003315003	2
	Clobetasol propionate	23D01-B01-228378	2
	Clobetasol propionate	23G04-B08-232382	1
	Clobetasol propionate	CLO001/0722	1
/Sanacorp	Clobetasol propionate	1804002-01	3
170420-01	Clobetasol propionate	17A057	1
20.12.2016 Phoenix 17,49EUR	Clobetasol propionate	15439504	1
AHC	Clobetasol propionate	1903014-01	5
AHC	Clobetasol propionate	23D01-B01-227673	1
AHD 14.06.19 Ek: 18,50	Clobetasol propionate	18082718	1
AHD	Clobetasol propionate	17E04-B02-338441	1
AHD	Clobetasol propionate	17L18-B02-347993	1
AHD	Clobetasol propionate	18/12-B02-35302	1
AHD	Clobetasol propionate	18/12-B02-355390	1
AHD	Clobetasol propionate	18/12-B02-357669	1
AHD	Clobetasol propionate	19j02-f02-3653202	1
AHD	Clobetasol propionate	20F24-F03-374147	1
AHD	Clobetasol propionate	21F11-B01	1
AHD	Clobetasol propionate	21L16-B08-221088	1
AHD	Clobetasol propionate	2209014-01	2
AHD	Clobetasol propionate	F02-3653202	1
AHD	Clobetasol propionate	F03-3741407	1
AHZ	Clobetasol propionate	1606022	1
Alliance H.	Clobetasol propionate	15234002	2
Alliance Health 17.0...	Clobetasol propionate	APBO0547/112010C	1
Alliance Healthcare	Clobetasol propionate	12J25-N01	1
Alliance Healthcare	Clobetasol propionate	18082714	1
Alliance Healthcare	Clobetasol propionate	18I12-B02-357669	1
Alliance Healthcare	Clobetasol propionate	1903014-01	3
Alliance Healthcare	Clobetasol propionate	21001700003	1
Alliance Healthcare	Clobetasol propionate	21001700007	1
Alliance Healthcare	Clobetasol propionate	21L16-B08-221090	1
Alliance	Clobetasol propionate	12342305	1
Alliance	Clobetasol propionate	21001700023	1
Allianz Healthcare 0...	Clobetasol propionate	1408018-01	1
Allianz Healthcare	Clobetasol propionate	18082709	1
allianz	Clobetasol propionate	15234009	1
Allianz	Clobetasol propionate	17325606	1
Anzag	Clobetasol propionate	1211021-02	1
Anzag	Clobetasol propionate	12E08-N04	1
Anzag	Clobetasol propionate	1408018-01	2
Anzag	Clobetasol propionate	15246001	1
Anzag	Clobetasol propionate	16106703	1
Anzag	Clobetasol propionate	192245012	1
Anzag	Clobetasol propionate	21001700003	1
Anzag	Clobetasol propionate	2109003-01	1
Anzag	Clobetasol propionate	CLO103/0220	1
apo-ident	Clobetasol propionate	1606022-01	2
apomix	Clobetasol propionate	1211021-03	1
apomix	Clobetasol propionate	16106703	1
apomix	Clobetasol propionate	16G18-B02-325571	1
apomix	Clobetasol propionate	200502501	2
Audor Pharma	Clobetasol propionate	ABCLP/M/036/16C	1
Audor Pharma	Clobetasol propionate	APAPL/035/E-12C	2
Audor Pharma	Clobetasol propionate	APB0054/112010C	1
Audor Pharma	Clobetasol propionate	APCLO102/0518C	8

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Audor Pharma	Clobetasol propionate	APCLP	1
Audor Pharma	Clobetasol propionate	APCLP/M/036/16C	5
Audor Pharma	Clobetasol propionate	APL/035/E-12C	1
Audor Pharma	Clobetasol propionate	APL035E12C	1
Audor Pharma	Clobetasol propionate	sieheBemerkung	1
Bombastus	Clobetasol propionate	12342303	1
Bombastus	Clobetasol propionate	13G23-N0	1
Bombastus	Clobetasol propionate	13G23-N01	1
Bombastus	Clobetasol propionate	1804002-01	2
Caelo	Clobetasol propionate		1
Caelo	Clobetasol propionate	1070317/16106704	1
Caelo	Clobetasol propionate	1105044-03	1
Caelo	Clobetasol propionate	1108044-02	1
Caelo	Clobetasol propionate	1108044-03	2
Caelo	Clobetasol propionate	1108044-04	1
Caelo	Clobetasol propionate	1110116	1
Caelo	Clobetasol propionate	11101311	1
Caelo	Clobetasol propionate	11101315	1
Caelo	Clobetasol propionate	11300702	3
Caelo	Clobetasol propionate	11300703	5
Caelo	Clobetasol propionate	11300707	2
Caelo	Clobetasol propionate	12107601	3
Caelo	Clobetasol propionate	12107602	3
Caelo	Clobetasol propionate	12107604	1
Caelo	Clobetasol propionate	12107606	1
Caelo	Clobetasol propionate	12107607	6
Caelo	Clobetasol propionate	12107608	1
Caelo	Clobetasol propionate	12107609	6
Caelo	Clobetasol propionate	121102104	1
Caelo	Clobetasol propionate	12342303	1
Caelo	Clobetasol propionate	12342306	6
Caelo	Clobetasol propionate	12342307	3
Caelo	Clobetasol propionate	12342308	1
Caelo	Clobetasol propionate	12342309	14
Caelo	Clobetasol propionate	12342310	7
Caelo	Clobetasol propionate	12342312	1
Caelo	Clobetasol propionate	123645	1
Caelo	Clobetasol propionate	12E08-N04	1
Caelo	Clobetasol propionate	12J25-N01	1
Caelo	Clobetasol propionate	13134701	17
Caelo	Clobetasol propionate	13134702	7
Caelo	Clobetasol propionate	13134703	4
Caelo	Clobetasol propionate	13134704	4
Caelo	Clobetasol propionate	13134705	4
Caelo	Clobetasol propionate	13269501	1
Caelo	Clobetasol propionate	13269502	3
Caelo	Clobetasol propionate	13269504	6
Caelo	Clobetasol propionate	13269505	2
Caelo	Clobetasol propionate	13269506	1
Caelo	Clobetasol propionate	13269507	3
Caelo	Clobetasol propionate	13269508	13
Caelo	Clobetasol propionate	13269509	1
Caelo	Clobetasol propionate	13269510	2
Caelo	Clobetasol propionate	1369504	1
Caelo	Clobetasol propionate	13A02-N04	1
Caelo	Clobetasol propionate	13G23-N01	1
Caelo	Clobetasol propionate	13K08-B30-287726	1
Caelo	Clobetasol propionate	13K08-B30-287728	1
Caelo	Clobetasol propionate	1408018-02	10
Caelo	Clobetasol propionate	1408018-03	10

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clobetasol propionate	14102416	1
Caelo	Clobetasol propionate	14188501	4
Caelo	Clobetasol propionate	14188502	6
Caelo	Clobetasol propionate	14188503	17
Caelo	Clobetasol propionate	14188504	7
Caelo	Clobetasol propionate	14188506	3
Caelo	Clobetasol propionate	14338001	9
Caelo	Clobetasol propionate	14338002	3
Caelo	Clobetasol propionate	14338005	3
Caelo	Clobetasol propionate	14338006	11
Caelo	Clobetasol propionate	14338007	6
Caelo	Clobetasol propionate	14338008	5
Caelo	Clobetasol propionate	1438007	1
Caelo	Clobetasol propionate	14C03-B07-293560	2
Caelo	Clobetasol propionate	14G30_B07_302114	1
Caelo	Clobetasol propionate	14G30-B07-302114	2
Caelo	Clobetasol propionate	14g30bo7302114	1
Caelo	Clobetasol propionate	15031401	1
Caelo	Clobetasol propionate	152340004	1
Caelo	Clobetasol propionate	15234001	11
Caelo	Clobetasol propionate	15234002	1
Caelo	Clobetasol propionate	15234003	19
Caelo	Clobetasol propionate	15234004	22
Caelo	Clobetasol propionate	15234008	1
Caelo	Clobetasol propionate	15234009	7
Caelo	Clobetasol propionate	1524003	1
Caelo	Clobetasol propionate	15246001	6
Caelo	Clobetasol propionate	15253032	1
Caelo	Clobetasol propionate	15412910	1
Caelo	Clobetasol propionate	154390504	1
Caelo	Clobetasol propionate	15439501	6
Caelo	Clobetasol propionate	15439502	8
Caelo	Clobetasol propionate	15439503	23
Caelo	Clobetasol propionate	15439504	27
Caelo	Clobetasol propionate	15439507	2
Caelo	Clobetasol propionate	1543953	1
Caelo	Clobetasol propionate	15A14-B02	1
Caelo	Clobetasol propionate	15C23-B02-310473	2
Caelo	Clobetasol propionate	15J-15-B04-316616	1
Caelo	Clobetasol propionate	15j15-b04-317698	1
Caelo	Clobetasol propionate	160115CP	1
Caelo	Clobetasol propionate	1606022	1
Caelo	Clobetasol propionate	160602201	1
Caelo	Clobetasol propionate	1606022-01	4
Caelo	Clobetasol propionate	1606022-02	6
Caelo	Clobetasol propionate	1606022-025349	1
Caelo	Clobetasol propionate	160829CP	1
Caelo	Clobetasol propionate	160919Di	1
Caelo	Clobetasol propionate	1610670	1
Caelo	Clobetasol propionate	16106701	5
Caelo	Clobetasol propionate	16106702	16
Caelo	Clobetasol propionate	16106703	22
Caelo	Clobetasol propionate	16106704	28
Caelo	Clobetasol propionate	16106709	21
Caelo	Clobetasol propionate	16106710	12
Caelo	Clobetasol propionate	16106711	26
Caelo	Clobetasol propionate	16106712	5
Caelo	Clobetasol propionate	16106713	6
Caelo	Clobetasol propionate	16106715	9
Caelo	Clobetasol propionate	16106718	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clobetasol propionate	16106719	6
Caelo	Clobetasol propionate	16106720	8
Caelo	Clobetasol propionate	16107704	1
Caelo	Clobetasol propionate	1616703	1
Caelo	Clobetasol propionate	1616715	1
Caelo	Clobetasol propionate	16348001	1
Caelo	Clobetasol propionate	16353208	1
Caelo	Clobetasol propionate	16C18-B02-325573	1
Caelo	Clobetasol propionate	16E04-B12	1
Caelo	Clobetasol propionate	16E04-B12-321034	4
Caelo	Clobetasol propionate	16E04-B12-321036	1
Caelo	Clobetasol propionate	16E04-B12-322020	2
Caelo	Clobetasol propionate	16G18-B02-324627	1
Caelo	Clobetasol propionate	16G18-B02-325572	1
Caelo	Clobetasol propionate	16H22-B07-328012	1
Caelo	Clobetasol propionate	1704020	1
Caelo	Clobetasol propionate	170402001	2
Caelo	Clobetasol propionate	1704020-01	17
Caelo	Clobetasol propionate	170404CP1606022-02	1
Caelo	Clobetasol propionate	17090708	1
Caelo	Clobetasol propionate	17096701	13
Caelo	Clobetasol propionate	17096702	9
Caelo	Clobetasol propionate	17096703	2
Caelo	Clobetasol propionate	17096704	5
Caelo	Clobetasol propionate	17096705	23
Caelo	Clobetasol propionate	17096706	24
Caelo	Clobetasol propionate	17096706/1180418	1
Caelo	Clobetasol propionate	17096707	16
Caelo	Clobetasol propionate	17096708	38
Caelo	Clobetasol propionate	17096709	12
Caelo	Clobetasol propionate	1709704	1
Caelo	Clobetasol propionate	17097608	1
Caelo	Clobetasol propionate	17325601	15
Caelo	Clobetasol propionate	17325602	39
Caelo	Clobetasol propionate	17325603	22
Ĉaelo	Clobetasol propionate	17325604	1
Caelo	Clobetasol propionate	17325605	20
Caelo	Clobetasol propionate	17325606	4
Caelo	Clobetasol propionate	17325607	1
Caelo	Clobetasol propionate	1735603	1
Caelo	Clobetasol propionate	17E04-B02-336882	1
Caelo	Clobetasol propionate	17g14	1
Caelo	Clobetasol propionate	17G14-B12-340176	1
Caelo	Clobetasol propionate	17G14-B12-341742	1
Caelo	Clobetasol propionate	17L18-B02-347993	1
Caelo	Clobetasol propionate	18/12-B02-353203	1
Caelo	Clobetasol propionate	18/12-B02-35480	1
Caelo	Clobetasol propionate	18/12-B02-355390	1
Caelo	Clobetasol propionate	18/12-b02-355657	1
Caelo	Clobetasol propionate	180400201	2
Caelo	Clobetasol propionate	1804002-01	14
Caelo	Clobetasol propionate	18040020108638392	1
Caelo	Clobetasol propionate	18082701	1
Caelo	Clobetasol propionate	18082702	14
Caelo	Clobetasol propionate	18082703	29
Caelo	Clobetasol propionate	18082708	27
Caelo	Clobetasol propionate	18082709	36
Caelo	Clobetasol propionate	18082710	21
Caelo	Clobetasol propionate	18082711	6
Caelo	Clobetasol propionate	18082714	14

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clobetasol propionate	18082717	6
Caelo	Clobetasol propionate	18082718	14
Caelo	Clobetasol propionate	180827708	1
Caelo	Clobetasol propionate	181016709	1
Caelo	Clobetasol propionate	1812B02355390	1
Caelo	Clobetasol propionate	183000204	2
Caelo	Clobetasol propionate	183000209	1
Caelo	Clobetasol propionate	183002001	5
Caelo	Clobetasol propionate	18300202	6
Caelo	Clobetasol propionate	18300203	18
Caelo	Clobetasol propionate	18300204	20
Caelo	Clobetasol propionate	18300204P-191206-1	1
Caelo	Clobetasol propionate	18300207	2
Caelo	Clobetasol propionate	18300208	20
Caelo	Clobetasol propionate	18300209	24
Caelo	Clobetasol propionate	18300210	27
Caelo	Clobetasol propionate	18300212	11
Caelo	Clobetasol propionate	18300213	18
Caelo	Clobetasol propionate	1830024	1
Caelo	Clobetasol propionate	18H22-B017-328012	1
Caelo	Clobetasol propionate	190301401	1
Caelo	Clobetasol propionate	1922245002	1
Caelo	Clobetasol propionate	192245002	19
Caelo	Clobetasol propionate	192245003	24
Caelo	Clobetasol propionate	192245004	25
Caelo	Clobetasol propionate	192245007	12
Caelo	Clobetasol propionate	192245009	16
Caelo	Clobetasol propionate	192245011	43
Caelo	Clobetasol propionate	192245012	16
Caelo	Clobetasol propionate	192245012/5020	1
Caelo	Clobetasol propionate	192245014	1
Caelo	Clobetasol propionate	192245015	14
Caelo	Clobetasol propionate	19224507	1
Caelo	Clobetasol propionate	19224514	1
Caelo	Clobetasol propionate	1922455004	1
Caelo	Clobetasol propionate	19300213	1
Caelo	Clobetasol propionate	19G23-B05-363805	1
Caelo	Clobetasol propionate	20004302002	17
Caelo	Clobetasol propionate	20004302003	49
Caelo	Clobetasol propionate	20004302004	1
Caelo	Clobetasol propionate	20004302006	11
Caelo	Clobetasol propionate	20004302009	18
Caelo	Clobetasol propionate	200043202009	1
Caelo	Clobetasol propionate	20043202003	1
Caelo	Clobetasol propionate	2005025-01	5
Caelo	Clobetasol propionate	20111700001	1
Caelo	Clobetasol propionate	20121012-4	1
Caelo	Clobetasol propionate	2014E-02835	1
Caelo	Clobetasol propionate	20F24-F03-374147	2
Caelo	Clobetasol propionate	21001700001	21
Caelo	Clobetasol propionate	21001700003	30
Caelo	Clobetasol propionate	21001700004	2
Caelo	Clobetasol propionate	21001700007	31
Caelo	Clobetasol propionate	21001700008	27
Caelo	Clobetasol propionate	2100170001	2
Caelo	Clobetasol propionate	21001700011	2
Caelo	Clobetasol propionate	21001700013	38
Caelo	Clobetasol propionate	21001700015	13
Caelo	Clobetasol propionate	21001700018	3
Caelo	Clobetasol propionate	21001700019	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clobetasol propionate	21001700021	11
Caelo	Clobetasol propionate	21001700023	1
Caelo	Clobetasol propionate	21001700025	3
Caelo	Clobetasol propionate	21001700026	7
Caelo	Clobetasol propionate	21001700027	2
Caelo	Clobetasol propionate	2100170003	3
Caelo	Clobetasol propionate	2100170013	1
Caelo	Clobetasol propionate	2100170015	1
Caelo	Clobetasol propionate	2100170026	1
Caelo	Clobetasol propionate	210170015	1
Caelo	Clobetasol propionate	23000426006	6
Caelo	Clobetasol propionate	23111202	1
Caelo	Clobetasol propionate	2778	1
Caelo	Clobetasol propionate	2829	1
Caelo	Clobetasol propionate	2x17325602	1
Caelo	Clobetasol propionate	3012Q02835	1
Caelo	Clobetasol propionate	31071302	1
Caelo	Clobetasol propionate	3110350	1
Caelo	Clobetasol propionate	3440	1
Caelo	Clobetasol propionate	36/AKD2	1
Caelo	Clobetasol propionate	4/0216	1
Caelo	Clobetasol propionate	5119U02835	1
Caelo	Clobetasol propionate	8082703	1
Caelo	Clobetasol propionate	apl/294/b-14	1
Caelo	Clobetasol propionate	CLO/1191217	1
Caelo	Clobetasol propionate	CLO004/0216	1
Caelo	Clobetasol propionate	CLO024/0915	1
Caeolo /Sana	Clobetasol propionate	18082711	1
Caeolo/Krieger	Clobetasol propionate	17096706	3
Caeolo/Noweda	Clobetasol propionate	15439503	1
Caeolo	Clobetasol propionate	17096709	1
Caesar & Loretz /Phönix	Clobetasol propionate	20004302003	1
Caesar & Loretz GmbH...	Clobetasol propionate	18300212	1
Caesar & Loretz GmbH...	Clobetasol propionate	18300210	1
Caesar & Loretz GmbH...	Clobetasol propionate	192245009	2
Caesar & Loretz GmbH...	Clobetasol propionate	18300204	1
Caesar & Loretz GmbH...	Clobetasol propionate	18300213	1
Caesar & Loretz GmbH...	Clobetasol propionate	18082718	1
Caesar & Loretz GmbH...	Clobetasol propionate	192245002	1
Caesar & Loretz GmbH...	Clobetasol propionate	192245011	1
Caesar & Loretz GmbH...	Clobetasol propionate	18082709	2
Caesar & Loretz GmbH...	Clobetasol propionate	192245002	2
Caesar & Loretz GmbH...	Clobetasol propionate	20004302003	1
Caesar & Loretz GmbH...	Clobetasol propionate	20004302009	1
Caesar & Loretz GmbH...	Clobetasol propionate	21001700007	1
Caesar & Loretz GmbH...	Clobetasol propionate	192245002	1
Caesar & Loretz GmbH...	Clobetasol propionate	192245011	2
Caesar & Loretz GmbH...	Clobetasol propionate	20004302003	1
Caesar & Loretz GmbH...	Clobetasol propionate	192245003	1
Caesar & Loretz GmbH...	Clobetasol propionate	21001700021	1
Caesar & Loretz GmbH/AEP	Clobetasol propionate	18300203	1
Caesar & Loretz GmbH/AHD	Clobetasol propionate	20004302009	1
Caesar & Loretz GmbH...	Clobetasol propionate	18082714	1
Caesar & Loretz GmbH...	Clobetasol propionate	18300204	1
Caesar & Loretz GmbH/G	Clobetasol propionate	20004302003	1
Caesar & Loretz GmbH/Gehe	Clobetasol propionate	18082702	1
Caesar & Loretz GmbH/Gehe	Clobetasol propionate	18082714	1
Caesar & Loretz GmbH/Gehe	Clobetasol propionate	192245002	1
Caesar & Loretz GmbH/Gehe	Clobetasol propionate	192245004	1
Caesar & Loretz GmbH/Gehe	Clobetasol propionate	20004302002	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Gehe	Clobetasol propionate	21001700008	1
Caesar & Loretz GmbH...	Clobetasol propionate	20004302004	1
Caesar & Loretz GmbH...	Clobetasol propionate	21001700013	1
Caesar & Loretz GmbH...	Clobetasol propionate	18300213	1
Caesar & Loretz GmbH...	Clobetasol propionate	192245002	1
Caesar & Loretz GmbH...	Clobetasol propionate	20004302003	1
Caesar & Loretz GmbH...	Clobetasol propionate	23000426001	1
Caesar & Loretz GmbH...	Clobetasol propionate	AP221112-02	1
Caesar & Loretz GmbH...	Clobetasol propionate	18300212	2
Caesar & Loretz GmbH/l10	Clobetasol propionate	21001700013	1
Caesar & Loretz GmbH...	Clobetasol propionate	192245004	2
Caesar & Loretz GmbH...	Clobetasol propionate	192245009	1
Caesar & Loretz GmbH...	Clobetasol propionate	192245012	2
Caesar & Loretz GmbH...	Clobetasol propionate	20004302009	2
Caesar & Loretz GmbH...	Clobetasol propionate	21001700001	1
Caesar & Loretz GmbH...	Clobetasol propionate	21001700008	1
Caesar & Loretz GmbH...	Clobetasol propionate	21001700015	1
Caesar & Loretz GmbH...	Clobetasol propionate	21001700021	1
Caesar & Loretz GmbH...	Clobetasol propionate	18300213	1
Caesar & Loretz GmbH...	Clobetasol propionate	20004302009	1
Caesar & Loretz GmbH...	Clobetasol propionate	18300204	2
Caesar & Loretz GmbH...	Clobetasol propionate	18300212	1
Caesar & Loretz GmbH...	Clobetasol propionate	192245007	1
Caesar & Loretz GmbH...	Clobetasol propionate	21001700003	1
Caesar & Loretz GmbH...	Clobetasol propionate	21001700007	1
Caesar & Loretz GmbH...	Clobetasol propionate	21001700013	1
Caesar & Loretz GmbH/Sana	Clobetasol propionate	21001700003	1
Caesar & Loretz GmbH...	Clobetasol propionate	18082709	1
Caesar & Loretz GmbH...	Clobetasol propionate	18300212	1
Caesar & Loretz GmbH...	Clobetasol propionate	192245003	1
Caesar & Loretz GmbH...	Clobetasol propionate	192245007	1
Caesar & Loretz GmbH...	Clobetasol propionate	192245011	1
Caesar & Loretz GmbH...	Clobetasol propionate	21001700013	2
Caesar & Loretz GmbH	Clobetasol propionate	16106702	3
Caesar & Loretz GmbH	Clobetasol propionate	18082703	1
Caesar & Loretz GmbH	Clobetasol propionate	18082708	4
Caesar & Loretz GmbH	Clobetasol propionate	18082709	8
Caesar & Loretz GmbH	Clobetasol propionate	18082710	4
Caesar & Loretz GmbH	Clobetasol propionate	18082711	1
Caesar & Loretz GmbH	Clobetasol propionate	18082714	4
Caesar & Loretz GmbH	Clobetasol propionate	18082718	6
Caesar & Loretz GmbH	Clobetasol propionate	183002001	3
Caesar & Loretz GmbH	Clobetasol propionate	18300202	2
Caesar & Loretz GmbH	Clobetasol propionate	18300203	2
Caesar & Loretz GmbH	Clobetasol propionate	18300204	12
Caesar & Loretz GmbH	Clobetasol propionate	18300208	8
Caesar & Loretz GmbH	Clobetasol propionate	18300209	9
Caesar & Loretz GmbH	Clobetasol propionate	18300210	5
Caesar & Loretz GmbH	Clobetasol propionate	18300212	5
Caesar & Loretz GmbH	Clobetasol propionate	18300213	6
Caesar & Loretz GmbH	Clobetasol propionate	192245002	10
Caesar & Loretz GmbH	Clobetasol propionate	192245003	10
Caesar & Loretz GmbH	Clobetasol propionate	192245004	5
Caesar & Loretz GmbH	Clobetasol propionate	192245005	1
Caesar & Loretz GmbH	Clobetasol propionate	192245007	7
Caesar & Loretz GmbH	Clobetasol propionate	192245009	5
Caesar & Loretz GmbH	Clobetasol propionate	192245011	19
Caesar & Loretz GmbH	Clobetasol propionate	192245012	4
Caesar & Loretz GmbH	Clobetasol propionate	192245015	2
Caesar & Loretz GmbH	Clobetasol propionate	20004302002	8

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Clobetasol propionate	20004302003	23
Caesar & Loretz GmbH	Clobetasol propionate	20004302006	4
Caesar & Loretz GmbH	Clobetasol propionate	20004302009	6
Caesar & Loretz GmbH	Clobetasol propionate	21001700001	6
Caesar & Loretz GmbH	Clobetasol propionate	21001700002	1
Caesar & Loretz GmbH	Clobetasol propionate	21001700003	9
Caesar & Loretz GmbH	Clobetasol propionate	21001700004	2
Caesar & Loretz GmbH	Clobetasol propionate	21001700007	4
Caesar & Loretz GmbH	Clobetasol propionate	21001700008	3
Caesar & Loretz GmbH	Clobetasol propionate	21001700011	2
Caesar & Loretz GmbH	Clobetasol propionate	21001700013	9
Caesar & Loretz GmbH	Clobetasol propionate	21001700015	5
Caesar & Loretz GmbH	Clobetasol propionate	21001700019	1
Caesar & Loretz GmbH	Clobetasol propionate	21001700021	3
Caesar & Loretz GmbH	Clobetasol propionate	21001700025	4
Caesar & Loretz GmbH	Clobetasol propionate	F02-3669403	1
Caesar & Loretz Hild...	Clobetasol propionate	192245002	1
Caesar & Loretz Hild...	Clobetasol propionate	192245003	1
Caesar & Loretz Hild...	Clobetasol propionate	192245011	1
Caesar & Loretz Hilden	Clobetasol propionate	18300204	1
Caesar & Loretz Hilden	Clobetasol propionate	18300213	1
Caesar & Loretz/ Noweda	Clobetasol propionate	12342306	1
Caesar & Loretz/AHD	Clobetasol propionate	192245003	1
Caesar & Loretz/Gehe	Clobetasol propionate	192245011	1
Caesar & Loretz/Geil...	Clobetasol propionate	20004302003	1
Caesar & Loretz/Noweda	Clobetasol propionate	20004302009	1
Caesar & Loretz	Clobetasol propionate	17096705	2
Caesar & Loretz	Clobetasol propionate	192245015	1
Caesar & Loretz	Clobetasol propionate	20004302002	1
Caesar Loretz	Clobetasol propionate	192245011	1
Caesar u Loretz	Clobetasol propionate	12107608	2
Caesar und Loretz	Clobetasol propionate	18300203	1
Caesar und Loretz	Clobetasol propionate	18300208	2
Caesar&Lorenz	Clobetasol propionate	1610370	1
Caesar&Lorenz	Clobetasol propionate	20004302002	1
Caesar&Loretz GmbH	Clobetasol propionate	15234001	1
Caesar&Loretz GmbH	Clobetasol propionate	15439501	1
Caesar&Loretz GmbH	Clobetasol propionate	192245015	1
Caesar/Lorenz	Clobetasol propionate	12342305	3
Caesar/Lorenz	Clobetasol propionate	12342309	1
Caesar/Loretz	Clobetasol propionate	12342310	1
Cealo /Gehe	Clobetasol propionate	18082710	1
Cealo	Clobetasol propionate	1408018	1
Cealo	Clobetasol propionate	16106702	2
cealo	Clobetasol propionate	16106703	1
Cealo	Clobetasol propionate	192245003	1
Cealo	Clobetasol propionate	21001700003	1
Chiesi/ Now	Clobetasol propionate	13269503	3
Crystal Pharma	Clobetasol propionate	C0054/1	1
Delta	Clobetasol propionate	17096701	1
DR.WOLFF	Clobetasol propionate	15J15-B04-317699	1
E Plus	Clobetasol propionate	16106702	1
eur	Clobetasol propionate	1704020-01	2
EuRho / Gehe	Clobetasol propionate	1903014-01	4
EuRho / Noweda	Clobetasol propionate	2109003-01	1
EuRho 06.10.2011 Anzag	Clobetasol propionate	1108044-01	1
EuRho- Phoenix	Clobetasol propionate	2109003-01	1
EuRho/ Anzag	Clobetasol propionate	29(1903014-01)	1
EuRho/ NOWEDA	Clobetasol propionate	1704020-01	1
EuRho/ NOWEDA	Clobetasol propionate	1804002-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho/ Phönix	Clobetasol propionate	1704020-01	1
EuRho/Fiebig	Clobetasol propionate	2005025-01	1
EuRho/Gehe	Clobetasol propionate	1704020-01	2
EuRho/Noveda	Clobetasol propionate	1804002-01	1
EuRho/Phoenix	Clobetasol propionate	160602202	1
EuRho/Phoenix	Clobetasol propionate	1903014	1
EuRho/Sanacorp	Clobetasol propionate	1704020-01	1
EuRho/Sanacorp	Clobetasol propionate	1903014-01	1
EuRho/Sanacorp	Clobetasol propionate	2005025-01	1
EuRho/Sanacorp	Clobetasol propionate	2109003-01	2
EuRho	Clobetasol propionate	1108044-04	2
EuRho	Clobetasol propionate	1408018-01	1
EuRho	Clobetasol propionate	1408018-02	2
EuRho	Clobetasol propionate	1704020-01	1
EuRho	Clobetasol propionate	1804002-01	2
EuRho	Clobetasol propionate	1903014-01	4
EuRho	Clobetasol propionate	2109003-01	1
euro AHD	Clobetasol propionate	1704020-015592	1
euro AHD	Clobetasol propionate	1804002-015788	1
Euro OCT / Krieger	Clobetasol propionate	1903014-01	1
Euro OT	Clobetasol propionate	14081018-02	1
Euro OTC	Clobetasol propionate	100402-01	1
Euro OTC	Clobetasol propionate	1072015D	1
Euro OTC	Clobetasol propionate	1105044-04	1
Euro OTC	Clobetasol propionate	1108044	1
Euro OTC	Clobetasol propionate	1108044-01	4
Euro OTC	Clobetasol propionate	1108044-02	8
Euro OTC	Clobetasol propionate	1108044-03	14
Euro OTC	Clobetasol propionate	1108044-037-16	1
Euro OTC	Clobetasol propionate	110804404	2
Euro OTC	Clobetasol propionate	1108044-04	15
Euro OTC	Clobetasol propionate	112/1018	1
Euro OTC	Clobetasol propionate	1204037-01	1
Euro OTC	Clobetasol propionate	12082013B	1
Euro OTC	Clobetasol propionate	12110-01	1
Euro OTC	Clobetasol propionate	1211021/02	1
Euro OTC	Clobetasol propionate	121102101	2
Euro OTC	Clobetasol propionate	1211021-01	20
Euro OTC	Clobetasol propionate	1211021-02	31
Euro OTC	Clobetasol propionate	1211021-03	30
Euro OTC	Clobetasol propionate	1211021-04	21
Euro OTC	Clobetasol propionate	121K021-01	1
Euro OTC	Clobetasol propionate	13042015A	1
Euro OTC	Clobetasol propionate	130604002	1
Euro OTC	Clobetasol propionate	13G23-N01	1
Euro OTC	Clobetasol propionate	1402018-03	1
Euro OTC	Clobetasol propionate	14080-02	1
Euro OTC	Clobetasol propionate	1408015-01	1
Euro OTC	Clobetasol propionate	1408018	1
Euro OTC	Clobetasol propionate	140801801	1
Euro OTC	Clobetasol propionate	1408018-01	17
Euro OTC	Clobetasol propionate	140801802	1
Euro OTC	Clobetasol propionate	1408018-02	78
Euro OTC	Clobetasol propionate	140801803	2
Euro OTC	Clobetasol propionate	1408018-03	32
Euro OTC	Clobetasol propionate	140808-02	1
Euro OTC	Clobetasol propionate	14080818-02	1
Euro OTC	Clobetasol propionate	15234003	1
Euro OTC	Clobetasol propionate	1601046-01	1
Euro OTC	Clobetasol propionate	16042014C	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Clobetasol propionate	1606022	3
Euro OTC	Clobetasol propionate	160602201	6
Euro OTC	Clobetasol propionate	1606022-01	32
Euro OTC	Clobetasol propionate	160602202	6
Euro OTC	Clobetasol propionate	1606022-02	62
Euro OTC	Clobetasol propionate	160622-02	1
Euro OTC	Clobetasol propionate	16106720	1
Euro OTC	Clobetasol propionate	1704020	2
Euro OTC	Clobetasol propionate	170402001	9
Euro OTC	Clobetasol propionate	1704020-01	142
Euro OTC	Clobetasol propionate	1704020-015498	1
Euro OTC	Clobetasol propionate	17044020-01	2
Euro OTC	Clobetasol propionate	17096705	1
Euro OTC	Clobetasol propionate	17096709	1
Euro OTC	Clobetasol propionate	171107CP/1704020-01	1
Euro OTC	Clobetasol propionate	17E04-B02-338441	1
Euro OTC	Clobetasol propionate	17L18-B02-347993	1
Euro OTC	Clobetasol propionate	18004002-01	1
Euro OTC	Clobetasol propionate	1801002-01	1
Euro OTC	Clobetasol propionate	180400002	1
Euro OTC	Clobetasol propionate	180400-01	1
Euro OTC	Clobetasol propionate	18040002-01	1
Euro OTC	Clobetasol propionate	1804001-01	1
Euro OTC	Clobetasol propionate	1804002	1
Euro OTC	Clobetasol propionate	180400201	5
Euro OTC	Clobetasol propionate	1804002-01	191
Euro OTC	Clobetasol propionate	1804002201	1
Euro OTC	Clobetasol propionate	1804002-41	1
Euro OTC	Clobetasol propionate	18041808	1
Euro OTC	Clobetasol propionate	18082703	2
Euro OTC	Clobetasol propionate	18082708	1
Euro OTC	Clobetasol propionate	18082709	1
Euro OTC	Clobetasol propionate	18082717	1
Euro OTC	Clobetasol propionate	18111403	1
Euro OTC	Clobetasol propionate	1903014	1
Euro OTC	Clobetasol propionate	190301401	5
Euro OTC	Clobetasol propionate	1903014-01	179
Euro OTC	Clobetasol propionate	19030414-01	1
Euro OTC	Clobetasol propionate	19031401	1
Euro OTC	Clobetasol propionate	191142210	1
Euro OTC	Clobetasol propionate	200025-01	1
Euro OTC	Clobetasol propionate	2003023-01	1
Euro OTC	Clobetasol propionate	2003026/01	2
Euro OTC	Clobetasol propionate	200302601	1
Euro OTC	Clobetasol propionate	2003026-01	10
Euro OTC	Clobetasol propionate	200502501	11
Euro OTC	Clobetasol propionate	2005025-01	121
Euro OTC	Clobetasol propionate	200505-01	1
Euro OTC	Clobetasol propionate	21001700008	2
Euro OTC	Clobetasol propionate	21090003-01	1
Euro OTC	Clobetasol propionate	210900301	4
Euro OTC	Clobetasol propionate	2109003-01	76
Euro OTC	Clobetasol propionate	2111I-02835	1
Euro OTC	Clobetasol propionate	220826(2005025-01)	1
Euro OTC	Clobetasol propionate	2209014-01	1
Euro OTC	Clobetasol propionate	2835	1
Euro OTC	Clobetasol propionate	30092014A	1
Euro OTC	Clobetasol propionate	31606022-02	1
Euro OTC	Clobetasol propionate	4091512	1
Euro OTC	Clobetasol propionate	4113Q-02835	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Clobetasol propionate	700225	2
Euro OTC	Clobetasol propionate	80616-1	1
Euro OTC	Clobetasol propionate	819081-39	1
Euro OTC	Clobetasol propionate	CLO105-0519	1
Euro OTC	Clobetasol propionate	CLO112/1018	2
Euro OTC	Clobetasol propionate	CLO119/1217	2
Euro OTC	Clobetasol propionate	Clob100123	1
Euro OTC	Clobetasol propionate	CLO-BL2153/0711	1
Euro OTC	Clobetasol propionate	CLO-BL2322/1012	2
Euro OTC	Clobetasol propionate	CLO-BLT223/1216	1
Euro OTC	Clobetasol propionate	clo-blt223/126	1
Euro OTC	Clobetasol propionate	EuroOTC	4
Euro OTC	Clobetasol propionate	P14091725/1606022-01	1
Euro/ANZAG	Clobetasol propionate	1606022-02	1
Euro/ANZAG	Clobetasol propionate	1804002-01	1
EuRo/Anzag	Clobetasol propionate	1804002-01	3
Euro/ANZAG	Clobetasol propionate	1903014-01	1
Euro/Phönix	Clobetasol propionate	210900301	1
euro/Symbiotica/Alli	Clobetasol propionate	1903014-01	1
Euro	Clobetasol propionate	1211021-02	2
EuRoh/ Gehe	Clobetasol propionate	1804002-01	2
euroho/gehe	Clobetasol propionate	1211021-01	1
EurRho/Noweda	Clobetasol propionate	2005025-01	1
Eurro/Phoenix	Clobetasol propionate	1804002-01	1
Fagon / Gehe	Clobetasol propionate	18/12-B02-354809	1
Fagron	Clobetasol propionate		1
Fagron	Clobetasol propionate	11/29-N07	1
Fagron	Clobetasol propionate	11-05-N06	1
Fagron	Clobetasol propionate	11300703	1
Fagron	Clobetasol propionate	11C16-NO1	1
Fagron	Clobetasol propionate	11D26-N04	1
Fagron	Clobetasol propionate	11H10-N02	1
Fagron	Clobetasol propionate	11L12-N05	2
Fagron	Clobetasol propionate	11129-N07	1
Fagron	Clobetasol propionate	1211021	1
Fagron	Clobetasol propionate	1211021-02	1
Fagron	Clobetasol propionate	12A02-N04	1
Fagron	Clobetasol propionate	12E08N04	1
Fagron	Clobetasol propionate	12E08-N04	11
Fagron	Clobetasol propionate	12J25-N01	5
Fagron	Clobetasol propionate	1314705	1
Fagron	Clobetasol propionate	13A02-N04	18
Fagron	Clobetasol propionate	13Ao2-N04	1
Fagron	Clobetasol propionate	13G23N01	1
Fagron	Clobetasol propionate	13G23-N01	18
Fagron	Clobetasol propionate	13G23-N01NT0421M	1
Fagron	Clobetasol propionate	13G23-NO1	1
Fagron	Clobetasol propionate	13K08-B03-287728	1
Fagron	Clobetasol propionate	13K08-B30	2
Fagron	Clobetasol propionate	13K08-B30-287726	2
Fagron	Clobetasol propionate	13K08B30287727	1
Fagron	Clobetasol propionate	13K08-B30-287727	2
Fagron	Clobetasol propionate	13-K08-B30-287727	1
Fagron	Clobetasol propionate	13k08b30287728	1
Fagron	Clobetasol propionate	13K08-B30-287728	6
Fagron	Clobetasol propionate	13K08-B30-287729	2
Fagron	Clobetasol propionate	13K08B30287730	1
Fagron	Clobetasol propionate	13K08-B30-287730	2
Fagron	Clobetasol propionate	1405018-02	1
Fagron	Clobetasol propionate	14188502	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clobetasol propionate	14C03-B07	3
Fagron	Clobetasol propionate	14C03-B07-293560	1
Fagron	Clobetasol propionate	14C03-B07-293561	2
Fagron	Clobetasol propionate	14C03-B07-293562	9
Fagron	Clobetasol propionate	14C03-B07-293563	2
Fagron	Clobetasol propionate	14C03-B07-305985	1
Fagron	Clobetasol propionate	14C03-B07-305986	2
Fagron	Clobetasol propionate	14C03-B07-305987	2
Fagron	Clobetasol propionate	14G30_B07_302112	1
Fagron	Clobetasol propionate	14G30-B07	1
Fagron	Clobetasol propionate	14G30-B07-302112	2
Fagron	Clobetasol propionate	14G30-B07-302113	2
Fagron	Clobetasol propionate	14G30-B07-302114	11
Fagron	Clobetasol propionate	14G30-B07-302115	2
Fagron	Clobetasol propionate	14G30B07-302116	1
Fagron	Clobetasol propionate	14G30-B07-302116	4
Fagron	Clobetasol propionate	14G30-B07-303114	1
Fagron	Clobetasol propionate	15/15-B04-317699	1
Fagron	Clobetasol propionate	15a14-b02-303125	2
Fagron	Clobetasol propionate	15A14-B02-303125	12
Fagron	Clobetasol propionate	15C23-B02_310473	2
Fagron	Clobetasol propionate	15c23-b02-310473	2
Fagron	Clobetasol propionate	15C23-B02-310473	12
Fagron	Clobetasol propionate	15C23-B02-310522	3
Fagron	Clobetasol propionate	15G01-B02-311578	1
Fagron	Clobetasol propionate	15H26-B03-312355	4
Fagron	Clobetasol propionate	15H26-B03-312860	1
Fagron	Clobetasol propionate	15J15-B04	1
Fagron	Clobetasol propionate	15J15-B04-316615	1
Fagron	Clobetasol propionate	15j15-B04-317698	1
Fagron	Clobetasol propionate	15J15-B04-317698	6
Fagron	Clobetasol propionate	15J15-B04-317699	1
Fagron	Clobetasol propionate	1606022-02	1
Fagron	Clobetasol propionate	16106704	1
Fagron	Clobetasol propionate	16E04-B12	1
Fagron	Clobetasol propionate	16E04-B12-321032	1
Fagron	Clobetasol propionate	16E04-B12-321033	3
Fagron	Clobetasol propionate	16E04-B12-321034	3
Fagron	Clobetasol propionate	16E04-B12-321035	1
Fagron	Clobetasol propionate	16E04-B12-321036	2
Fagron	Clobetasol propionate	16E04-B12-322020	4
Fagron	Clobetasol propionate	16G18-B02-324627	6
Fagron	Clobetasol propionate	16G18B02325571	1
Fagron	Clobetasol propionate	16G18-B02-325571	2
Fagron	Clobetasol propionate	16G18-B02-325572	1
Fagron	Clobetasol propionate	16G18-B02-325573	8
Fagron	Clobetasol propionate	16G18-B02-32571	1
Fagron	Clobetasol propionate	16H22-B07	1
Fagron	Clobetasol propionate	16H22-B07-328012	14
Fagron	Clobetasol propionate	16H22-B07-330169	3
Fagron	Clobetasol propionate	16K24-B04	2
Fagron	Clobetasol propionate	16K24-B04-331220	1
Fagron	Clobetasol propionate	16k24-b04-332086	1
Fagron	Clobetasol propionate	16K24-B04-332086	6
Fagron	Clobetasol propionate	16K24-B04-333120	6
Fagron	Clobetasol propionate	16K24B04333121	1
Fagron	Clobetasol propionate	16K24-B04-333121	3
Fagron	Clobetasol propionate	16K24-B04-333143	5
Fagron	Clobetasol propionate	16K24-B04-333120	1
Fagron	Clobetasol propionate	170402001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clobetasol propionate	1704020-01	4
Fagron	Clobetasol propionate	17096708	1
Fagron	Clobetasol propionate	17E04B02335335	1
Fagron	Clobetasol propionate	17E04-B02-335335	5
Fagron	Clobetasol propionate	17E04B02336882	1
Fagron	Clobetasol propionate	17E04-B02-336882	2
Fagron	Clobetasol propionate	17e04-b02-338441	1
Fagron	Clobetasol propionate	17E04-B02-338441	6
Fagron	Clobetasol propionate	17G14-B12	1
Fagron	Clobetasol propionate	17G14-B12-340175	6
Fagron	Clobetasol propionate	17G14-B12-340176	3
Fagron	Clobetasol propionate	17G14-B12-341742	1
Fagron	Clobetasol propionate	17g14-b12-341743	1
Fagron	Clobetasol propionate	17G14-B12-341743	3
Fagron	Clobetasol propionate	17L18-B02	3
Fagron	Clobetasol propionate	17L18B02-344841	1
Fagron	Clobetasol propionate	17L18-B02-344841	3
Fagron	Clobetasol propionate	17L18-B02-344842	3
Fagron	Clobetasol propionate	17L18-B02-345403	7
Fagron	Clobetasol propionate	17L18-B02-345404	4
Fagron	Clobetasol propionate	17L18B02347991	1
Fagron	Clobetasol propionate	17L18-B02347991	1
Fagron	Clobetasol propionate	17L18-B02-347991	1
Fagron	Clobetasol propionate	17L18-B02-347992	4
Fagron	Clobetasol propionate	17l18-b02-347993	1
Fagron	Clobetasol propionate	17L18-B02-347993	7
Fagron	Clobetasol propionate	17L18-B02-351867	3
Fagron	Clobetasol propionate	17LK18-B02-344841	1
Fagron	Clobetasol propionate	18/12-B02_357669	1
Fagron	Clobetasol propionate	18/12-b02-0002	1
Fagron	Clobetasol propionate	18/12-B02-353201	5
Fagron	Clobetasol propionate	18/12-B02-353202	8
Fagron	Clobetasol propionate	18/12-B02-353203	1
Fagron	Clobetasol propionate	18/12-B02-354809	2
Fagron	Clobetasol propionate	18/12-B02-355065	1
Fagron	Clobetasol propionate	18/12-B02-355390	3
Fagron	Clobetasol propionate	18/12-B02-355657	3
Fagron	Clobetasol propionate	18/12-B02-357670	1
Fagron	Clobetasol propionate	18/12-BO2-353202	2
Fagron	Clobetasol propionate	18/12-BO2-354809	1
Fagron	Clobetasol propionate	1804002-01	1
Fagron	Clobetasol propionate	18112-B02-357669	1
Fagron	Clobetasol propionate	1812-B02-353202	1
Fagron	Clobetasol propionate	1812-B02-353203	1
Fagron	Clobetasol propionate	18I12-02	1
Fagron	Clobetasol propionate	18I12-B02	5
Fagron	Clobetasol propionate	18I12-B02_357670	1
Fagron	Clobetasol propionate	18I12-B02-353202	4
Fagron	Clobetasol propionate	18I12-B02-353203	3
Fagron	Clobetasol propionate	18I12-B02-355065	1
Fagron	Clobetasol propionate	18I12-B02-355390	4
Fagron	Clobetasol propionate	18I12-B02-355391	4
Fagron	Clobetasol propionate	18I12-B02-357669	3
Fagron	Clobetasol propionate	18I12-B02-357670	1
Fagron	Clobetasol propionate	18I12-BO2-355391	1
Fagron	Clobetasol propionate	18l12-B02-353202	1
Fagron	Clobetasol propionate	18l12-B02-353203	1
Fagron	Clobetasol propionate	18l12-B02-354809	1
Fagron	Clobetasol propionate	18l12-B02-355065	1
Fagron	Clobetasol propionate	18l12-B02-355657	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clobetasol propionate	18112-B02-357669	1
Fagron	Clobetasol propionate	18112-Bo2-353201	1
Fagron	Clobetasol propionate	19/L10F02-366943	1
Fagron	Clobetasol propionate	1903014-01	1
Fagron	Clobetasol propionate	19B06-B03	2
Fagron	Clobetasol propionate	19B06-B03-360420	1
Fagron	Clobetasol propionate	19B06-B03-360421	4
Fagron	Clobetasol propionate	19B06-B03-360426	1
Fagron	Clobetasol propionate	19b06-b03-360603	1
Fagron	Clobetasol propionate	19B06-B03-360603	1
Fagron	Clobetasol propionate	19B06-B03-60603	1
Fagron	Clobetasol propionate	19G23_B05_363805	1
Fagron	Clobetasol propionate	19G23-B05	3
Fagron	Clobetasol propionate	19G23-B05-363804	3
Fagron	Clobetasol propionate	19G23-B05-363805	6
Fagron	Clobetasol propionate	19G23-B05-363806	11
Fagron	Clobetasol propionate	19G23-B05-363808	2
Fagron	Clobetasol propionate	19G23-B05-363806	1
Fagron	Clobetasol propionate	19J02-F02	3
Fagron	Clobetasol propionate	19J02-F02-365320	4
Fagron	Clobetasol propionate	19J02-F02-365321	6
Fagron	Clobetasol propionate	19J02F02-365322	1
Fagron	Clobetasol propionate	19J02-F02365322	1
Fagron	Clobetasol propionate	19J02-F02-365322	11
Fagron	Clobetasol propionate	19J02-F02-365324	4
Fagron	Clobetasol propionate	19JO2-F02-365322	1
Fagron	Clobetasol propionate	19L10-F02	1
Fagron	Clobetasol propionate	19L10-F02-3669402	1
Fagron	Clobetasol propionate	19L10-F02-366941	6
Fagron	Clobetasol propionate	19L10F02366942	1
Fagron	Clobetasol propionate	19L10-F02-366942	7
Fagron	Clobetasol propionate	19L10-F02-366942CLO113/0619	1
Fagron	Clobetasol propionate	19L10F02366943	2
Fagron	Clobetasol propionate	19L10-F02-366943	10
Fagron	Clobetasol propionate	19L10-F02-366945	1
Fagron	Clobetasol propionate	20F24-F03-374147	8
Fagron	Clobetasol propionate	20F24-F03-374148	3
Fagron	Clobetasol propionate	20F-24-F03-374148	1
Fagron	Clobetasol propionate	21F11-B01-213854	5
Fagron	Clobetasol propionate	21f11-b01-217282	1
Fagron	Clobetasol propionate	21F11-B01-217282	4
Fagron	Clobetasol propionate	21L16-B08-216942	1
Fagron	Clobetasol propionate	21L16-B08-218980	2
Fagron	Clobetasol propionate	21L16-B08-221088	4
Fagron	Clobetasol propionate	21L16-B08-216879	1
Fagron	Clobetasol propionate	21L6B08	1
Fagron	Clobetasol propionate	22H25B08	1
Fagron	Clobetasol propionate	22L20-B03-227672	1
Fagron	Clobetasol propionate	341743	1
Fagron	Clobetasol propionate	3713M-02835	1
Fagron	Clobetasol propionate	B05-3638004	1
Fagron	Clobetasol propionate	B05-3638006	1
Fagron	Clobetasol propionate	B05-3680006	1
Fagron	Clobetasol propionate	CLO001/0421	1
Fagron	Clobetasol propionate	CLO002/0621	2
Fagron	Clobetasol propionate	CLO101/0417	1
Fagron	Clobetasol propionate	Clo103/0220	1
Fagron	Clobetasol propionate	CLO103/0220	1
Fagron	Clobetasol propionate	CLO103/0518	3
Fagron	Clobetasol propionate	CLO105/0519	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clobetasol propionate	CLO111/1018	2
Fagron	Clobetasol propionate	CLO113/0619	5
Fagron	Clobetasol propionate	CLO4645878	1
Fagron	Clobetasol propionate	F02-3653202	2
Fagron	Clobetasol propionate	F02-3669401	1
Fagron	Clobetasol propionate	F02-3669403	2
Fagron	Clobetasol propionate	NS0292-M	1
Fagron	Clobetasol propionate	NS0486M	1
Fagron	Clobetasol propionate	NT0421M	3
Fargon/Phoenix 23.01.2018	Clobetasol propionate	17E04-B02-338441	1
Fargon	Clobetasol propionate	14C03-B07	1
Farmabios / Gehe	Clobetasol propionate	15234003	1
Farmabios / Gehe	Clobetasol propionate	18082703	1
Farmabios S.p.A./Cae...	Clobetasol propionate	14338006	1
Farmabios S.p.A.	Clobetasol propionate	18300204	1
Farmabios S.p.A/AHD	Clobetasol propionate	18082708	1
Farmabios S.p.A/AHD	Clobetasol propionate	18082718	1
Fgaron	Clobetasol propionate	15H26-B03	1
fgron Services B.V./ Gehe	Clobetasol propionate	F02-3669401	1
Fiebig	Clobetasol propionate	1804002-01	1
Finteler Apotheke	Clobetasol propionate	16K24-B04-333121	2
Fischar	Clobetasol propionate	14188506	1
GEHE 21.03.2014	Clobetasol propionate	1211021-02	1
Gehe amax	Clobetasol propionate	15439501	1
Gehe amax	Clobetasol propionate	18300204	1
Gehe/Euroh	Clobetasol propionate	190301401	1
Gehe	Clobetasol propionate	10D21-N04	1
Gehe	Clobetasol propionate	12107606	1
Gehe	Clobetasol propionate	12342306	2
Gehe	Clobetasol propionate	12342310	1
Gehe	Clobetasol propionate	12J25-N01	1
Gehe	Clobetasol propionate	1408018-02	1
Gehe	Clobetasol propionate	1408018-03	1
Gehe	Clobetasol propionate	14188504	1
Gehe	Clobetasol propionate	15234003	1
Gehe	Clobetasol propionate	1606022-01	2
Gehe	Clobetasol propionate	16106701	1
Gehe	Clobetasol propionate	16106704	1
GEHE	Clobetasol propionate	16G18-B02-324627	1
Gehe	Clobetasol propionate	170402001	1
Gehe	Clobetasol propionate	1704020-01	1
Gehe	Clobetasol propionate	17096705	1
GEHE	Clobetasol propionate	17096707	1
Gehe	Clobetasol propionate	17096708	1
Gehe	Clobetasol propionate	1804002-01	1
GEHE	Clobetasol propionate	18082702	1
Gehe	Clobetasol propionate	18082703	1
Gehe	Clobetasol propionate	183002001	2
Gehe	Clobetasol propionate	18I12-B02-353203	1
Gehe	Clobetasol propionate	18I12-B02-355391	1
Gehe	Clobetasol propionate	1903014-01	2
Gehe	Clobetasol propionate	20004302009	1
GEHE	Clobetasol propionate	210017000003	1
Gehe	Clobetasol propionate	21001700013	1
Gehe	Clobetasol propionate	21001700018	1
Gehe	Clobetasol propionate	21001700025	2
Gehe	Clobetasol propionate	2100700026	1
Gehe	Clobetasol propionate	2109003-01	1
GEHE	Clobetasol propionate	2209014_01	1
Gehe	Clobetasol propionate	2209014-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
GEHE	Clobetasol propionate	22H25-B08-223090	1
Gehe	Clobetasol propionate	23000426002	2
Gehe	Clobetasol propionate	23000426003	1
Gehe	Clobetasol propionate	23003315001	1
gehe	Clobetasol propionate	APCLPM03616C	1
gehe	Clobetasol propionate	Fagron23D-01B01-227673	1
Geilenkirchen	Clobetasol propionate	18082703	1
Geilenkirchen	Clobetasol propionate	192245011	1
Geilenkirchen	Clobetasol propionate	210017000003	1
HCK	Clobetasol propionate	11/05-N06	1
Hedinger/ Sanacorp	Clobetasol propionate	APAPL/035/E-12C	1
Hedinger	Clobetasol propionate	1704020-01	1
Henry Lamotte	Clobetasol propionate	16106704	1
Heyl/Noweda	Clobetasol propionate	15234001	2
Ichtyol / Noweda	Clobetasol propionate	17325605	1
Jenapharm/Noweda	Clobetasol propionate	15234004	1
Jenne	Clobetasol propionate	17325601	2
Jenne	Clobetasol propionate	21001700001	1
Jenne	Clobetasol propionate	21001700013	5
Jenne	Clobetasol propionate	22H25-B0B-225386	1
Kehr	Clobetasol propionate	22000315001	1
Kehr	Clobetasol propionate	23000426001	1
Kehr	Clobetasol propionate	2300042600214	1
Krieger	Clobetasol propionate	2209014-01	1
L10	Clobetasol propionate	16106703	2
L10	Clobetasol propionate	18082708	1
L12	Clobetasol propionate	16106711	1
L12	Clobetasol propionate	17325602	1
Midas	Clobetasol propionate	16106704	2
Midas	Clobetasol propionate	17096705	1
Nachprüfung vom 19.06.17	Clobetasol propionate	9302004	2
Nachprüfung	Clobetasol propionate	2082019-11	1
Newchem / Gehe	Clobetasol propionate	17096708	1
Newchem S.p.A./Link	Clobetasol propionate	NZ0263M/X2835	1
Newchem S.p.A.	Clobetasol propionate	192245008	1
Newchem/Phoenix	Clobetasol propionate	NZ0263M	2
Newchem	Clobetasol propionate	15439504	2
Noweda /Cealo	Clobetasol propionate	18300209	1
Noweda 6.4.17	Clobetasol propionate	1606022-01	1
Noweda/ Ichthyol	Clobetasol propionate	15439503	1
Noweda/Anzag	Clobetasol propionate	13269504	3
Noweda/EuRo	Clobetasol propionate	1606022-01	1
Noweda	Clobetasol propionate	11300702	1
Noweda	Clobetasol propionate	12342305	1
Noweda	Clobetasol propionate	12342310	1
Noweda	Clobetasol propionate	13134701	1
Noweda	Clobetasol propionate	13134705	1
Noweda	Clobetasol propionate	14338007	1
Noweda	Clobetasol propionate	15234004	1
Noweda	Clobetasol propionate	1606022-02	1
Noweda	Clobetasol propionate	16106720	1
Noweda	Clobetasol propionate	17096706	1
Noweda	Clobetasol propionate	17325605	1
Noweda	Clobetasol propionate	17G14-B12-340175	1
Noweda	Clobetasol propionate	1804002-01	2
Noweda	Clobetasol propionate	18300202	1
Noweda	Clobetasol propionate	18300204	1
Noweda	Clobetasol propionate	18300208	1
Noweda	Clobetasol propionate	18300213	1
Noweda	Clobetasol propionate	1903014-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Clobetasol propionate	192245003	1
Noweda	Clobetasol propionate	20004302006	1
Noweda	Clobetasol propionate	2005025-01	3
Noweda	Clobetasol propionate	21001700003	1
Noweda	Clobetasol propionate	21001700023	1
Noweda	Clobetasol propionate	21001700025	1
Noweda	Clobetasol propionate	2109003-01	3
Noweda	Clobetasol propionate	2209014-01	1
Noweda	Clobetasol propionate	22H25-B08-223090	1
Noweda	Clobetasol propionate	23000426001	2
NOWEDA	Clobetasol propionate	23000426001	1
Oberlinden Apotheke	Clobetasol propionate	B0054/116010Mg60g	1
Parthe Apotheke	Clobetasol propionate	96/21	1
Ph.Eur 8.0	Clobetasol propionate	16106709	1
Phoenix 02.04.2014	Clobetasol propionate	1211021-03	3
Phoenix 24.11.2017	Clobetasol propionate	17096706	1
Phoenix 29.11.12	Clobetasol propionate	700225	2
Phoenix WE 29.04.17 ...	Clobetasol propionate	1606022-02	1
Phoenix/Cealo	Clobetasol propionate	17096701	1
phoenix/fargon	Clobetasol propionate	17L18-B02-345403	1
Phoenix	Clobetasol propionate	13K08B30287728	1
Phoenix	Clobetasol propionate	15439502	1
Phoenix	Clobetasol propionate	16h22-b07-328012	1
Phoenix	Clobetasol propionate	16H-B07-330169	1
Phoenix	Clobetasol propionate	1704020-01	1
Phoenix	Clobetasol propionate	1804002-01	1
Phoenix	Clobetasol propionate	18082703	2
Phoenix	Clobetasol propionate	18082709	1
Phoenix	Clobetasol propionate	183002001	1
Phoenix	Clobetasol propionate	1903014-01	2
Phoenix	Clobetasol propionate	192245002	1
Phoenix	Clobetasol propionate	192245011	1
Phoenix	Clobetasol propionate	20004302002	1
Phoenix	Clobetasol propionate	20004302003	2
Phoenix	Clobetasol propionate	200451305	1
Phoenix	Clobetasol propionate	21001700007	1
Phoenix	Clobetasol propionate	2100170003	1
Phoenix	Clobetasol propionate	2109003-01	1
Phoenix	Clobetasol propionate	2209014-01	1
Phoenix	Clobetasol propionate	22H25-B08-223090	1
Phoenix	Clobetasol propionate	23000426001	3
Phoenix	Clobetasol propionate	23000426003	1
Phoenix	Clobetasol propionate	3063	1
Phoenix	Clobetasol propionate	3365	1
Phoenix	Clobetasol propionate	3366	1
Phönix Caesar u. Loretz	Clobetasol propionate	13269508	1
Phönix Gotha	Clobetasol propionate	1108044-04	1
Phönix Gotha	Clobetasol propionate	1211021-02	3
Phönix Gotha	Clobetasol propionate	18082708	1
phönix herne	Clobetasol propionate	180400201	1
Phönix, Caesar&Loret...	Clobetasol propionate	18300213	1
Phönix/Apo-Ident	Clobetasol propionate	1606022-02	1
Phönix/Euro	Clobetasol propionate	1804002-01	1
Phönix	Clobetasol propionate		1
Phönix	Clobetasol propionate	1211021-04	1
Phönix	Clobetasol propionate	13134701	1
phönix	Clobetasol propionate	15439503	1
phönix	Clobetasol propionate	15439504	1
Phönix	Clobetasol propionate	15H26-B03-312860	1
Phönix	Clobetasol propionate	16106703	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
phönix	Clobetasol propionate	16106704	1
Phönix	Clobetasol propionate	17096706	2
Phönix	Clobetasol propionate	1804002-01	1
phönix	Clobetasol propionate	18082703	1
Phönix	Clobetasol propionate	18300204	1
Phönix	Clobetasol propionate	192245004	1
Phönix	Clobetasol propionate	20004302002	1
Phönix	Clobetasol propionate	2002025-01	1
Phönix	Clobetasol propionate	200990910	1
Phönix	Clobetasol propionate	21001700026	1
Phönix	Clobetasol propionate	2109003-01	1
Phönix	Clobetasol propionate	3161	1
Phönix	Clobetasol propionate	3182	1
Phönix	Clobetasol propionate	F02-3653202	1
PhönixWE24.10.2014 ...	Clobetasol propionate	1211021-04	1
Raben-Apotheke Mildenau	Clobetasol propionate	13k08-b30-287727	1
Röntgen	Clobetasol propionate	1804002-01	1
Sanacorp	Clobetasol propionate	1108044-03	1
Sanacorp	Clobetasol propionate	12107608	1
Sanacorp	Clobetasol propionate	12107609	2
Sanacorp	Clobetasol propionate	1211021-01	1
Sanacorp	Clobetasol propionate	12342310	1
Sanacorp	Clobetasol propionate	13269507	1
sanacorp	Clobetasol propionate	13269508	1
Sanacorp	Clobetasol propionate	13g23n01	1
sanacorp	Clobetasol propionate	14188506	1
Sanacorp	Clobetasol propionate	15234003	1
Sanacorp	Clobetasol propionate	1606022-02	2
Sanacorp	Clobetasol propionate	18082708	1
Sanacorp	Clobetasol propionate	18300204	1
Sanacorp	Clobetasol propionate	18I12-B02_357669	1
Sanacorp	Clobetasol propionate	192245004	1
Sanacorp	Clobetasol propionate	20004302009	1
Sanacorp	Clobetasol propionate	2005025-01	1
Sanacorp	Clobetasol propionate	21001700003	2
Sanacorp	Clobetasol propionate	21001700023	1
Sanacorp	Clobetasol propionate	21L16-B08-221088	1
Sanacorp	Clobetasol propionate	230003315003	1
Sanacorp	Clobetasol propionate	23000426001	2
sanacorp	Clobetasol propionate	23000426002	1
Sanacorp;19.03.15;87,60EUR	Clobetasol propionate	14C03-B07-293563	1
Symbiotica / Gehe	Clobetasol propionate	1408018-02	1
Symbiotica / Gehe	Clobetasol propionate	1408018-03	2
Symbiotica / Noweda	Clobetasol propionate	1704020-01	1
Symbiotica Spec. Ing...	Clobetasol propionate	19J02-F02-365322	1
Symbiotica Spec./Phönix	Clobetasol propionate	1108044-04	1
Symbiotica Spec./Phönix	Clobetasol propionate	CLO-B12153/0711	1
Symbiotica Spec.	Clobetasol propionate	1211021-03	1
symbiotica/gehe	Clobetasol propionate	1211021-03	1
Symbiotica/Noweda	Clobetasol propionate	CLO119/1217	1
Symbiotica/Phönix	Clobetasol propionate	1408018-02	1
Symbiotica/Sanacorp	Clobetasol propionate	1408018-03	1
Symbiotica	Clobetasol propionate	2005025-01	2
symbiotica	Clobetasol propionate	2109003	1
Symbiotica	Clobetasol propionate	2109003-01	1
Symbiotitica/Noweda	Clobetasol propionate	1606022-01	1
VDL	Clobetasol propionate	2109003-01	1
WE: 20.01.16	Clobetasol propionate	15234004	1

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 231 623 spectra from 1513 *Apo-Ident* customers from a total of 48 653 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Clobetasol propionate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Clobetasol propionate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	740	0	152 222
Type B	0	1184	0	200 900
Type C	0	4346	98	231 623

The substance/substance group *Clobetasol propionate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1892 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4932 %)
Type C	100.0000 % (> 99.9007 %)	97.7948 % (> 97.7273 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21092	21092	0.00	75.82
21473	21473	0.00	55.71
21611	21611	0.00	54.44
21802	21802	0.00	114.52
21896	21896	0.00	79.38
22714	22714	0.00	54.21
22724	21092	5.98	74.93
24691	25349	8.08	53.48
24904	24904	0.00	80.40
25349	25349	0.00	52.73

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Clonidine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20637-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Clonidine hydrochloride; Clonidini hydrochloridum

Special notes

When selecting the *Clonidine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Clonidine hydrochloride	6	4	11

Second-stage model

For differentiation of the substance/substance group *Clonidine hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Clonidine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	123.39	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Clonidine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Clonidine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Clonidine hydrochloride	13I25-B07	21220	40	20131009
Fagron	Clonidine hydrochloride	14H11-B04-311163	21966	60	AR-18-FG-006797-02
Fagron	Clonidine hydrochloride	14H11-B04-311163	22967	40	20140929
Fagron	Clonidine hydrochloride	14H11-B04-311163	22967SI	40	20140929
Fagron	Clonidine hydrochloride	19B27-B02-361777	24687	40	20190607
Fagron	Clonidine hydrochloride	22A26-B04-216708	26141	40	20220316
Fagron	Clonidine hydrochloride	22A26-B04-216708	26141SI	40	20220316
Fagron	Clonidine hydrochloride	22B22-B03-216999	26142	40	20220505
Fagron	Clonidine hydrochloride	22B22-B03-216999	26142SI	40	20220505
Fagron	Clonidine hydrochloride	24A29-B05-234630	27186	40	20240227

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 420 spectra of 10 reference samples from the substance/substance group *Clonidine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

samples come from 6 different batches.

- 152 542 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 540 spectra of 13 reference samples from the substance/substance group *Clonidine hydrochloride*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Clonidine hydrochloride	15L11-B01-332270	23228	40
Fagron	Clonidine hydrochloride	18B12-B04-353341	24443	40
Fagron	Clonidine hydrochloride	20D29-F02-374142	25785	40
Fagron	Clonidine hydrochloride	21F07-B03-213617	25907	40
Fagron	Clonidine hydrochloride	14H11-B04-311163	21966SI†	60
Fagron	Clonidine hydrochloride	15L11-B01-332270	23228SI	40
Fagron	Clonidine hydrochloride	15L11-B01-332270	23410	40
Fagron	Clonidine hydrochloride	15L11-B01-332270	23410SI	40
Fagron	Clonidine hydrochloride	18B12-B04-353341	24443SI	40
Fagron	Clonidine hydrochloride	19B27-B02-361777	24687SI†	40
Fagron	Clonidine hydrochloride	20D29-F02-374142	25785SI	40
Fagron	Clonidine hydrochloride	21F07-B03-213617	25907SI	40
Fagron	Clonidine hydrochloride	24A29-B05-234630	27186SI†	40

- 201 544 spectra from a total of 4038 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 56 spectra from 18 *Apo-Ident* customers from 12 batches from the substance/substance group *Clonidine hydrochloride*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Clonidine hydrochloride	22B22-B03-225373	1
Fagron	Clonidine hydrochloride	14H11-B04-298642	1
Fagron	Clonidine hydrochloride	14H11-B04-311163	42
Fagron	Clonidine hydrochloride	15L11-B01	1
Fagron	Clonidine hydrochloride	18B12-B04-353341	1
Fagron	Clonidine hydrochloride	20D29-F02-3705608	1
Fagron	Clonidine hydrochloride	20D29-F02-370567	1
Fagron	Clonidine hydrochloride	21F07-B03-213617	1
Fagron	Clonidine hydrochloride	22B22-B03-217792	1
Fagron	Clonidine hydrochloride	22B22-B03-221078	2
Fagron	Clonidine hydrochloride	22B22-B03-225373	1
Fagron	Clonidine hydrochloride	77543E004	1
Fagron	Clonidine hydrochloride	F02-370567	1
Regenbogen Apotheke	Clonidine hydrochloride	18B12-B04-353341	1

- 236 011 spectra from 1515 *Apo-Ident* customers from a total of 49 246 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Clonidine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Clonidine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	540	0	201 544
Type C	0	56	0	236 011

The substance/substance group *Clonidine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8889 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 89.2857 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21220	21966	21.49	209.07
21966	21966	0.00	230.46
22967	21966	29.57	206.71
24687	21966	34.96	207.22
26141	21966	32.84	207.07
26142	21966	40.04	208.88
27186	21966	47.04	209.34

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Clotrimazole**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20000-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Clotrimazole; Clotrimazolum

Special notes

When selecting the *Clotrimazole* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Clotrimazole	12	15	881

Second-stage model

For differentiation of the substance/substance group *Clotrimazole* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Clotrimazole* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Bifonazole	42.54	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Clotrimazole* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Clotrimazole*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Clotrimazole	13184113	21087	40	20130614
Caelo	Clotrimazole	13224204	21114	40	20130815
Caelo	Clotrimazole	13224220	21352	40	20130815
Caelo	Clotrimazole	13224220	21353	40	20130815
Caelo	Clotrimazole	153956	23791	40	20151215*
Caelo	Clotrimazole	21000121	25649	40	20210330*
Caelo	Clotrimazole	21000123	25656	40	20210330*
Euro OTC	Clotrimazole	1306036-01	21207	40	20130823
Euro OTC	Clotrimazole	1510003	22229	60	20151111*
Fagron	Clotrimazole	12I21-N01	20794	40	20120322
Fagron	Clotrimazole	14B05-B36	21259	40	20140225
Fagron	Clotrimazole	14C04-B31	21264	40	20140319
Fagron	Clotrimazole	22A21-B02-217361	26137	40	20220411

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 540 spectra of 13 reference samples from the substance/substance group *Clotrimazole*. These samples are listed above in the *calibration samples* section. The reference samples come from 12 different batches.

- 152 422 spectra from a total of 2830 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 640 spectra of 18 reference samples from the substance/substance group *Clotrimazole*.

- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Clotrimazole	12320815	20861	30
Caelo	Clotrimazole	171116	23322	40
Caelo	Clotrimazole	17111616	23781	40
Caelo	Clotrimazole	190161	24512	40
Caelo	Clotrimazole	190162	24517	40
Caelo	Clotrimazole	21004117	26001	40
Caelo	Clotrimazole	23001597	26834	40
Euro OTC	Clotrimazole	1607046	22793	40
Euro OTC	Clotrimazole	1703028	23129	40
Euro OTC	Clotrimazole	1808028	24298	40
Euro OTC	Clotrimazole	1902004	24461	40
Euro OTC	Clotrimazole	2007033	25300	40
Euro OTC	Clotrimazole	2103024	25672	40
Euro OTC	Clotrimazole	2301055	26582	40
Euro OTC	Clotrimazole	2406013	27400	40
Caelo	Clotrimazole	21004117	26001SI	10
Euro OTC	Clotrimazole	2301055	26582SI	20
Fagron	Clotrimazole	22A21-B02-217361	26137SI†	20

- 201 444 spectra from a total of 4029 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6943 spectra from 1318 *Apo-Ident* customers from 933 batches from the substance/substance group *Clotrimazole*.
- Among them are spectra of independent samples from 878 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Clotrimazole	1306036-01	1
	Clotrimazole	14C04-B30-291661	1
	Clotrimazole	20H26-F05	1
	Clotrimazole	20H26-F05-373737	1
	Clotrimazole	20H26-F05-373738	1
	Clotrimazole	21000123010	1
	Clotrimazole	2100411016	1
	Clotrimazole	210041160007	1
	Clotrimazole	21004116005	5
	Clotrimazole	21004116007	9
	Clotrimazole	21004116008	2
	Clotrimazole	21004116012	1
	Clotrimazole	21004116013	3
	Clotrimazole	21004116014	21
	Clotrimazole	21004116016	4
	Clotrimazole	21004116017	1
	Clotrimazole	21004117004	1
	Clotrimazole	21004117005	1
	Clotrimazole	2100411701	1
	Clotrimazole	21004117011	1
	Clotrimazole	21004117013	1
	Clotrimazole	21004117016	2
	Clotrimazole	21004117017	7
	Clotrimazole	21004117018	15
	Clotrimazole	21004117019	6
	Clotrimazole	21004117022	9
	Clotrimazole	21004117023	2
	Clotrimazole	2100416016	1
	Clotrimazole	2103024-01	1
	Clotrimazole	2103024-02	8
	Clotrimazole	2103024-03	4
	Clotrimazole	214116014	1
	Clotrimazole	21D22-B03	1
	Clotrimazole	21D22-B03-217092	2
	Clotrimazole	21i24_b11_213292	1
	Clotrimazole	21I24-B11	1
	Clotrimazole	21I24-B11-213292	2
	Clotrimazole	22A21-B02-217361	1
	Clotrimazole	22A21-B02-217510	1
	Clotrimazole	22A21-B02-221730	2
	Clotrimazole	22A21-B02-221731	1
	Clotrimazole	22G29-B05-228695	1
	Clotrimazole	23001596002	19

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Clotrimazole	23001596003	4
	Clotrimazole	23001596008	3
	Clotrimazole	23001596009	5
	Clotrimazole	23001596010	3
	Clotrimazole	23003390001	1
	Clotrimazole	23003390004	1
	Clotrimazole	23003390005	1
	Clotrimazole	2301055_01	1
	Clotrimazole	23010550-01	1
	Clotrimazole	2301055-01	17
	Clotrimazole	2301055-02	10
	Clotrimazole	23D11-B01-228693	1
	Clotrimazole	23H09-B07-230826	1
	Clotrimazole	B11-2186308	1
	Clotrimazole	caelo	1
	Clotrimazole	HCZ20120	1
A.H.D.	Clotrimazole	14337801	1
AHC	Clotrimazole	23001596009	1
AHD 27.10 Ek.7,07	Clotrimazole	1607046	1
AHD/EuRho	Clotrimazole	1902004-01	1
AHD/Euro	Clotrimazole	1808028-02	1
AHD/Hedinger	Clotrimazole	14337807	1
AHD	Clotrimazole	13184105	1
AHD	Clotrimazole	14144914	1
AHD	Clotrimazole	16J07-B02-335773	1
AHD	Clotrimazole	16J07-B02-344817	1
AHD	Clotrimazole	1703028-03	1
AHD	Clotrimazole	1808028-01	1
AHD	Clotrimazole	18A18-B05-352114	1
AHD	Clotrimazole	190200-02	2
AHD	Clotrimazole	1902004-01	1
AHD	Clotrimazole	19B14-B01-359538	1
AHD	Clotrimazole	21004116008	1
AHD	Clotrimazole	21004116016	1
AHD	Clotrimazole	21004117023	1
AHD	Clotrimazole	2103024-02	1
AHD	Clotrimazole	2103024-03	1
AHD	Clotrimazole	22A21-B02-221730	1
AHD	Clotrimazole	23H09-B07-235135	1
Alliance Healthcare	Clotrimazole	1309034-01	1
Alliance Healthcare	Clotrimazole	18147216	1
Alliance Healthcare	Clotrimazole	21004117001	1
Alliance Healthcare	Clotrimazole	AP1510003-01C	1
Alliance	Clotrimazole	21004117011	1
Allianz Healthcare	Clotrimazole	18g10-b06-355382	1
Amoli / Gehe	Clotrimazole	CLT/1505/0016B	2
Amoli Organics Plot ...	Clotrimazole	17J25-Bo6-349161	1
Anzag	Clotrimazole	14C04-B30-2916618	1
Anzag	Clotrimazole	15395610	1
Anzag	Clotrimazole	15G14-B06	1
Anzag	Clotrimazole	1703028-01	1
Anzag	Clotrimazole	2007033-02	1
Anzag	Clotrimazole	2301055-04	1
apo ident	Clotrimazole	1607046-02	1
apo-ident	Clotrimazole	1902004-03	1
ApoIdent	Clotrimazole	2103024-1	1
Apo-klent	Clotrimazole	2103024-02	1
apomix	Clotrimazole	14B05-B36	1
apomix	Clotrimazole	15G14-B05-311100	1
apomix	Clotrimazole	15G14-B05-311103	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Audor Pharma	Clotrimazole	1703/0016CC	1
Audor Pharma	Clotrimazole	1703028-02	1
Audor Pharma	Clotrimazole	2007033-01	1
Audor Pharma	Clotrimazole	2007033-02	1
Audor Pharma	Clotrimazole	AP1306036-01C	1
Audor Pharma	Clotrimazole	APCL/1703/0016C	1
Audor Pharma	Clotrimazole	APCLT/1703/0016C	2
Audor Pharma	Clotrimazole	APCLT/1703/0016CC	4
Beiersdorf	Clotrimazole	15395611	1
Bombastus	Clotrimazole	1210039/02	1
Bombastus	Clotrimazole	12320815	1
Bombastus	Clotrimazole	14337817	1
Bombastus	Clotrimazole	1607046-01	2
Bombastus	Clotrimazole	17360203	1
Bombastus	Clotrimazole	18147211	1
Bombastus	Clotrimazole	Validierungsmessung	1
Caeelo / Gehe	Clotrimazole	18147211	1
cael	Clotrimazole	19016208	2
Caello/Anzag	Clotrimazole	14337815	1
Caelo	Clotrimazole		10
Caelo	Clotrimazole	10147203	1
Caelo	Clotrimazole	10247328	3
Caelo	Clotrimazole	1070716	1
Caelo	Clotrimazole	108/AKD1	1
Caelo	Clotrimazole	11/22-N10	1
Caelo	Clotrimazole	1105014-02	1
Caelo	Clotrimazole	11081201	1
Caelo	Clotrimazole	11305506	2
Caelo	Clotrimazole	11305507	1
Caelo	Clotrimazole	11305511	1
Caelo	Clotrimazole	11305513	8
Caelo	Clotrimazole	1150817/16234512	1
Caelo	Clotrimazole	1170717	1
Caelo	Clotrimazole	11-K21-N19	1
Caelo	Clotrimazole	1210030-02	1
Caelo	Clotrimazole	1210039-01	1
Caelo	Clotrimazole	12159902	11
Caelo	Clotrimazole	12159904	2
Caelo	Clotrimazole	12159911	2
Caelo	Clotrimazole	12159913	9
Caelo	Clotrimazole	12159916	6
Caelo	Clotrimazole	12320805	4
Caelo	Clotrimazole	12320806	5
Caelo	Clotrimazole	12320807	4
Caelo	Clotrimazole	12320808	11
Caelo	Clotrimazole	12320809	4
Caelo	Clotrimazole	12320813	3
Caelo	Clotrimazole	12320814	9
Caelo	Clotrimazole	12320815	1
Caelo	Clotrimazole	1234567	1
Caelo	Clotrimazole	1259913	1
Caelo	Clotrimazole	12B27-N05	2
Caelo	Clotrimazole	12E02-N12	2
Caelo	Clotrimazole	12E30-N07	1
Caelo	Clotrimazole	12I21-N04	1
Caelo	Clotrimazole	1306036	1
Caelo	Clotrimazole	130603601	1
Caelo	Clotrimazole	1306036-01	4
Caelo	Clotrimazole	1309034-02	3
Caelo	Clotrimazole	1309034-C1	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clotrimazole	13148007	1
Caelo	Clotrimazole	13184103	10
Caelo	Clotrimazole	13184105	13
Caelo	Clotrimazole	13184111	7
Caelo	Clotrimazole	131841111	1
Caelo	Clotrimazole	13184113	2
Caelo	Clotrimazole	132234216	1
Caelo	Clotrimazole	1322401	1
Caelo	Clotrimazole	13224201	21
Caelo	Clotrimazole	13224204	2
Caelo	Clotrimazole	13224210	11
Caelo	Clotrimazole	13224211	5
Caelo	Clotrimazole	13224212	8
Caelo	Clotrimazole	13224214	9
Caelo	Clotrimazole	13224215	3
Caelo	Clotrimazole	13224216	9
Caelo	Clotrimazole	13224217	9
Caelo	Clotrimazole	13224218	12
Caelo	Clotrimazole	13224219	7
Caelo	Clotrimazole	13224220	6
Caelo	Clotrimazole	13224221	2
Caelo	Clotrimazole	13224225	2
Caelo	Clotrimazole	132243218	1
Caelo	Clotrimazole	13324204	1
Caelo	Clotrimazole	1409027-02	2
Caelo	Clotrimazole	1409027-03	3
Caelo	Clotrimazole	1409027-04	1
Caelo	Clotrimazole	14101716	1
Caelo	Clotrimazole	141104C	1
Caelo	Clotrimazole	14144905	17
Caelo	Clotrimazole	14144911	13
Caelo	Clotrimazole	14144912	2
Caelo	Clotrimazole	14144913	2
Caelo	Clotrimazole	14144914	8
Caelo	Clotrimazole	14144917	5
Caelo	Clotrimazole	14144918	12
Caelo	Clotrimazole	143337811	1
Caelo	Clotrimazole	14337801	14
Caelo	Clotrimazole	14337802	8
Caelo	Clotrimazole	14337807	12
Caelo	Clotrimazole	14337809	14
Caelo	Clotrimazole	14337811	4
Caelo	Clotrimazole	14337812	7
Caelo	Clotrimazole	14337813	8
Caelo	Clotrimazole	14337814	9
Caelo	Clotrimazole	14337815	10
Caelo	Clotrimazole	14337816	17
Caelo	Clotrimazole	14337817	17
Caelo	Clotrimazole	14337818	14
Caelo	Clotrimazole	14337819	8
Caelo	Clotrimazole	14337824	3
Caelo	Clotrimazole	14337824NP	1
Caelo	Clotrimazole	14337827	10
Caelo	Clotrimazole	14337828	13
Caelo	Clotrimazole	14337829	20
Caelo	Clotrimazole	14337830	3
Caelo	Clotrimazole	14337832	1
Caelo	Clotrimazole	14338712	1
Caelo	Clotrimazole	1437816	1
Caelo	Clotrimazole	14B05-B35	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clotrimazole	14B05-B36-291167	1
Caelo	Clotrimazole	14B05-B36-291168	1
Caelo	Clotrimazole	14c04-b30-291656	1
Caelo	Clotrimazole	14C04-B30-291656	2
Caelo	Clotrimazole	14c04-B31	1
Caelo	Clotrimazole	14C04-B31-294939	1
Caelo	Clotrimazole	14c04-b31-299954	2
Caelo	Clotrimazole	14C04B31-299954	1
Caelo	Clotrimazole	14C04-B31-299955	1
Caelo	Clotrimazole	14C04-B32-291657	1
Caelo	Clotrimazole	1510003-01	4
Caelo	Clotrimazole	15295603	1
Caelo	Clotrimazole	15395602	20
Caelo	Clotrimazole	15395603	10
Caelo	Clotrimazole	15395604	15
Caelo	Clotrimazole	15395605	15
Caelo	Clotrimazole	1539561	1
Caelo	Clotrimazole	15395610	7
Caelo	Clotrimazole	15395611	13
Caelo	Clotrimazole	15395613	8
Caelo	Clotrimazole	15395614	8
Caelo	Clotrimazole	15395615	8
Caelo	Clotrimazole	15395617	12
Caelo	Clotrimazole	15395618	20
Caelo	Clotrimazole	15395618I-81216/1	1
Caelo	Clotrimazole	15395623	2
Caelo	Clotrimazole	1539613	1
Caelo	Clotrimazole	153965604	1
Caelo	Clotrimazole	156546	1
Caelo	Clotrimazole	15G14-B05-311101	1
Caelo	Clotrimazole	15G14-B05-311103	2
Caelo	Clotrimazole	15G14-B05-316483	2
Caelo	Clotrimazole	15G14-B06-311054	1
Caelo	Clotrimazole	15G14-B06-311057	1
Caelo	Clotrimazole	16051913	1
Caelo	Clotrimazole	160614	1
Caelo	Clotrimazole	160704601	1
Caelo	Clotrimazole	1607046-01	7
Caelo	Clotrimazole	1607046-02	7
Caelo	Clotrimazole	16131901	1
Caelo	Clotrimazole	1623417	1
Caelo	Clotrimazole	16234501	8
Caelo	Clotrimazole	16234502	6
Caelo	Clotrimazole	16234503	19
Caelo	Clotrimazole	16234504	11
Caelo	Clotrimazole	16234505	30
Caelo	Clotrimazole	16234506	1
Caelo	Clotrimazole	16234509	11
Caelo	Clotrimazole	16234511	20
Caelo	Clotrimazole	16234512	19
Caelo	Clotrimazole	16234513	26
Caelo	Clotrimazole	162345135319	1
Caelo	Clotrimazole	16234515	1
Caelo	Clotrimazole	16234517	10
Caelo	Clotrimazole	16234520	25
Caelo	Clotrimazole	16234521	11
Caelo	Clotrimazole	16234522	23
Caelo	Clotrimazole	162345225555	1
Caelo	Clotrimazole	16234523	1
Caelo	Clotrimazole	16234525	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clotrimazole	1623455	1
Caelo	Clotrimazole	16B09-B06-3115007	1
Caelo	Clotrimazole	16B09B06311506	1
Caelo	Clotrimazole	16B09-B06-311785	1
Caelo	Clotrimazole	16B11-B04-320088	1
Caelo	Clotrimazole	16B11-B04-322393	1
Caelo	Clotrimazole	16B11-B04-325221	1
Caelo	Clotrimazole	16E20-B10	2
Caelo	Clotrimazole	16E20-B10-324555	1
Caelo	Clotrimazole	16J07-B02	1
Caelo	Clotrimazole	16J07-B02_330236	1
Caelo	Clotrimazole	16J07-B02-329385	4
Caelo	Clotrimazole	16J07-B02-329386	1
Caelo	Clotrimazole	16J07-B02-330216	2
Caelo	Clotrimazole	16J07-B02-335773	1
Caelo	Clotrimazole	16J07-B02-344817	1
Caelo	Clotrimazole	16J07-B02-344818	2
Caelo	Clotrimazole	17/25-B06-345048	1
Caelo	Clotrimazole	17011601	1
Caelo	Clotrimazole	1703028	1
Caelo	Clotrimazole	170302801	4
Caelo	Clotrimazole	1703028-01	12
Caelo	Clotrimazole	1703028-02	4
Caelo	Clotrimazole	170302803	1
Caelo	Clotrimazole	1703028-03	4
Caelo	Clotrimazole	1703028-0318147206	1
Caelo	Clotrimazole	17053186	1
Caelo	Clotrimazole	171113608	1
Caelo	Clotrimazole	17111601	15
Caelo	Clotrimazole	17111603	4
Caelo	Clotrimazole	17111604	8
Caelo	Clotrimazole	17111605	19
Caelo	Clotrimazole	17111606	30
Caelo	Clotrimazole	17111608	12
Caelo	Clotrimazole	1711161	1
Caelo	Clotrimazole	17111612	1
Caelo	Clotrimazole	17111613	27
Caelo	Clotrimazole	17111615	27
Caelo	Clotrimazole	17111616	35
Caelo	Clotrimazole	17111617	5
Caelo	Clotrimazole	1711603	2
Caelo	Clotrimazole	1711604	2
Caelo	Clotrimazole	1711605	1
Caelo	Clotrimazole	1711606	2
Caelo	Clotrimazole	1711613	2
Caelo	Clotrimazole	1711816	1
Caelo	Clotrimazole	17260204	1
Caelo	Clotrimazole	1736002001	1
Caelo	Clotrimazole	173600201	2
Caelo	Clotrimazole	17360023	1
Caelo	Clotrimazole	17360201	30
Caelo	Clotrimazole	17360202	36
Caelo	Clotrimazole	17360203	16
Caelo	Clotrimazole	17360204	29
Caelo	Clotrimazole	17A19-B04	1
Caelo	Clotrimazole	17A19-B04-332097	1
Caelo	Clotrimazole	17A19-B04-340476	1
Caelo	Clotrimazole	17J25-B06-345045	1
Caelo	Clotrimazole	17J25-B06-345048	1
Caelo	Clotrimazole	17J25-B06-347476	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clotrimazole	18016104	1
Caelo	Clotrimazole	1808028-01	8
Caelo	Clotrimazole	1808028-02	5
Caelo	Clotrimazole	18081408	1
Caelo	Clotrimazole	1814211	1
Caelo	Clotrimazole	18147101	47
Caelo	Clotrimazole	18147102	41
Caelo	Clotrimazole	18147103	24
Caelo	Clotrimazole	181471035763	1
Caelo	Clotrimazole	18147201	2
Caelo	Clotrimazole	18147202	2
Caelo	Clotrimazole	18147203	38
Caelo	Clotrimazole	18147206	1
Caelo	Clotrimazole	18147208	2
Caelo	Clotrimazole	18147210	56
Caelo	Clotrimazole	18147211	49
Caelo	Clotrimazole	18147212	13
Caelo	Clotrimazole	18147215	3
Caelo	Clotrimazole	18147216	7
Caelo	Clotrimazole	18147217	8
Caelo	Clotrimazole	1847103	1
Caelo	Clotrimazole	1882321	2
Caelo	Clotrimazole	1882404	1
Caelo	Clotrimazole	18A18-B05-347865	2
Caelo	Clotrimazole	18A18-B05-348429	1
Caelo	Clotrimazole	18A18-B05-349662	1
Caelo	Clotrimazole	18A18B05350778	1
Caelo	Clotrimazole	18A18-B05-350780	1
Caelo	Clotrimazole	18A18-B05-350781	1
Caelo	Clotrimazole	18A18-b05-352115	1
Caelo	Clotrimazole	18A18-B05-352115	1
Caelo	Clotrimazole	18A18-B05-353892	1
Caelo	Clotrimazole	18A18-B056-352115	1
Caelo	Clotrimazole	18G10-B06-352425	1
Caelo	Clotrimazole	18G10-B06-352427	2
Caelo	Clotrimazole	18g10-b06-358825	1
Caelo	Clotrimazole	190016207	1
Caelo	Clotrimazole	19015107	1
Caelo	Clotrimazole	190160106	1
Caelo	Clotrimazole	1901606	1
Caelo	Clotrimazole	19016103	19
Caelo	Clotrimazole	19016104	17
Caelo	Clotrimazole	19016105	29
Caelo	Clotrimazole	19016106	27
Caelo	Clotrimazole	19016107	27
Caelo	Clotrimazole	19016108	17
Caelo	Clotrimazole	19016115	1
Caelo	Clotrimazole	19016115P-191111-1	1
Caelo	Clotrimazole	19016116	29
Caelo	Clotrimazole	19016119	23
Caelo	Clotrimazole	190162001	2
Caelo	Clotrimazole	19016202	20
Caelo	Clotrimazole	19016203	22
Caelo	Clotrimazole	19016204	23
Caelo	Clotrimazole	19016205	12
Caelo	Clotrimazole	19016206	16
Caelo	Clotrimazole	19016207	1
Caelo	Clotrimazole	19016208	25
Caelo	Clotrimazole	19016210	2
Caelo	Clotrimazole	19016212	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clotrimazole	190200401	1
Caelo	Clotrimazole	1902004-01	4
Caelo	Clotrimazole	19052401	1
Caelo	Clotrimazole	1906106	1
Caelo	Clotrimazole	190652002	1
Caelo	Clotrimazole	1916202	1
Caelo	Clotrimazole	192004-03	1
Caelo	Clotrimazole	19B14-B01	1
Caelo	Clotrimazole	19B14-B01-359537	1
Caelo	Clotrimazole	19B14-B01-359539	2
Caelo	Clotrimazole	19J23-F06-367382	1
Caelo	Clotrimazole	200000	1
Caelo	Clotrimazole	200000000094008	1
Caelo	Clotrimazole	200000092005	1
Caelo	Clotrimazole	200000094003	1
Caelo	Clotrimazole	200000094004	2
Caelo	Clotrimazole	2000002005	1
Caelo	Clotrimazole	2000004002	1
Caelo	Clotrimazole	200000892006	1
Caelo	Clotrimazole	2000009	1
Caelo	Clotrimazole	20000092002	16
Caelo	Clotrimazole	20000092005	10
Caelo	Clotrimazole	20000092006	24
Caelo	Clotrimazole	20000092007	26
Caelo	Clotrimazole	2000009202	1
Caelo	Clotrimazole	2000009207	1
Caelo	Clotrimazole	20000094001	1
Caelo	Clotrimazole	20000094002	24
Caelo	Clotrimazole	20000094003	25
Caelo	Clotrimazole	200000940033	1
Caelo	Clotrimazole	20000094004	33
Caelo	Clotrimazole	20000094005	35
Caelo	Clotrimazole	20000094006	26
Caelo	Clotrimazole	2000094006018824 04	1
Caelo	Clotrimazole	20000094007	1
Caelo	Clotrimazole	20000094008	20
Caelo	Clotrimazole	20000094009	1
Caelo	Clotrimazole	20000094012	1
Caelo	Clotrimazole	2000009404	2
Caelo	Clotrimazole	2000009408	1
Caelo	Clotrimazole	200003904005	1
Caelo	Clotrimazole	2000092002	1
Caelo	Clotrimazole	2000092006	1
Caelo	Clotrimazole	2000092007	1
Caelo	Clotrimazole	2000094003	1
Caelo	Clotrimazole	2000094004	1
Caelo	Clotrimazole	2000094005	1
Caelo	Clotrimazole	2000094008	3
Caelo	Clotrimazole	200009402	1
Caelo	Clotrimazole	20003904003	17
Caelo	Clotrimazole	20003904004	36
Caelo	Clotrimazole	20003904005	9
Caelo	Clotrimazole	20003904008	7
Caelo	Clotrimazole	2007033-01	4
Caelo	Clotrimazole	2007033-02	1
Caelo	Clotrimazole	2007033-03	1
Caelo	Clotrimazole	20111018	1
Caelo	Clotrimazole	20111115	1
Caelo	Clotrimazole	20160801	5
Caelo	Clotrimazole	2092	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clotrimazole	20H26F05373737	1
Caelo	Clotrimazole	21/24-B11-218638	1
Caelo	Clotrimazole	210000121002	1
Caelo	Clotrimazole	21000121002	43
Caelo	Clotrimazole	21000121003	27
Caelo	Clotrimazole	21000121004	47
Caelo	Clotrimazole	21000121005	2
Caelo	Clotrimazole	21000121006	24
Caelo	Clotrimazole	21000121008	13
Caelo	Clotrimazole	21000121009	28
Caelo	Clotrimazole	21000121010	29
Caelo	Clotrimazole	210001210101	1
Caelo	Clotrimazole	21000121013	15
Caelo	Clotrimazole	21000123006	17
Caelo	Clotrimazole	21000123008	23
Caelo	Clotrimazole	21000123010	9
Caelo	Clotrimazole	21000123011	17
Caelo	Clotrimazole	21000211006	1
Caelo	Clotrimazole	210004116005	1
Caelo	Clotrimazole	2100117013	1
Caelo	Clotrimazole	2100121009	1
Caelo	Clotrimazole	21004116001	12
Caelo	Clotrimazole	21004116003	7
Caelo	Clotrimazole	21004116005	9
Caelo	Clotrimazole	21004116006	3
Caelo	Clotrimazole	21004116007	2
Caelo	Clotrimazole	21004116008	1
Caelo	Clotrimazole	21004116013	2
Caelo	Clotrimazole	21004116014	3
Caelo	Clotrimazole	21004117001	12
Caelo	Clotrimazole	21004117003	3
Caelo	Clotrimazole	21004117004	9
Caelo	Clotrimazole	21004117005	10
Caelo	Clotrimazole	21004117007	19
Caelo	Clotrimazole	21004117011	2
Caelo	Clotrimazole	21004117013	1
Caelo	Clotrimazole	21004117016	9
Caelo	Clotrimazole	21004117017	5
Caelo	Clotrimazole	21004117018	5
Caelo	Clotrimazole	21004117019	1
Caelo	Clotrimazole	21004117022	2
Caelo	Clotrimazole	2100417005	1
Caelo	Clotrimazole	2103024-01	3
Caelo	Clotrimazole	210302402	2
Caelo	Clotrimazole	2103024-03	1
Caelo	Clotrimazole	21-24-B11-218638	1
Caelo	Clotrimazole	2217Q-01276	1
Caelo	Clotrimazole	23001596002	1
Caelo	Clotrimazole	26071305	1
Caelo	Clotrimazole	310316-5-461	1
Caelo	Clotrimazole	311111	1
Caelo	Clotrimazole	3335	1
Caelo	Clotrimazole	3456575	1
Caelo	Clotrimazole	412091-2-P	1
Caelo	Clotrimazole	415050-2-P	1
Caelo	Clotrimazole	418072-1-P	1
Caelo	Clotrimazole	5117E-01276	1
Caelo	Clotrimazole	54292100012113	1
Caelo	Clotrimazole	700135-0006	1
Caelo	Clotrimazole	8638446	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Clotrimazole	94006	1
Caelo	Clotrimazole	94008	1
Caelo	Clotrimazole	AP1510003-01C	1
Caelo	Clotrimazole	Fagron	1
Caelo	Clotrimazole	HCZ14218	1
Caelo	Clotrimazole	HCZ20120	1
Caelo	Clotrimazole	P-21091821/18147203	1
Caelo	Clotrimazole	PC85	1
Caeolo/Gehe	Clotrimazole	16234521	1
Caesar & Lorenz GmbH	Clotrimazole	21004117016	1
Caesar & Loretz /Phönix	Clotrimazole	2000094004	1
Caesar & Loretz GmbH...	Clotrimazole	21004117007	1
Caesar & Loretz GmbH...	Clotrimazole	21000121009	1
Caesar & Loretz GmbH...	Clotrimazole	19016108	1
Caesar & Loretz GmbH...	Clotrimazole	20000092006	1
Caesar & Loretz GmbH...	Clotrimazole	200000094005	1
Caesar & Loretz GmbH...	Clotrimazole	21000123008	1
Caesar & Loretz GmbH...	Clotrimazole	19016202	2
Caesar & Loretz GmbH...	Clotrimazole	19016103	1
Caesar & Loretz GmbH...	Clotrimazole	21000121009	1
Caesar & Loretz GmbH Sana	Clotrimazole	21004117011	1
Caesar & Loretz GmbH...	Clotrimazole	18147203	1
Caesar & Loretz GmbH...	Clotrimazole	20000094003	3
Caesar & Loretz GmbH...	Clotrimazole	20003904004	1
Caesar & Loretz GmbH...	Clotrimazole	20000094003	1
Caesar & Loretz GmbH...	Clotrimazole	21000123006	1
Caesar & Loretz GmbH...	Clotrimazole	20000092006	1
Caesar & Loretz GmbH...	Clotrimazole	20000094002	1
Caesar & Loretz GmbH...	Clotrimazole	20000094003	1
Caesar & Loretz GmbH...	Clotrimazole	20003904003	1
Caesar & Loretz GmbH...	Clotrimazole	21000121004	1
Caesar & Loretz GmbH...	Clotrimazole	19016205	1
Caesar & Loretz GmbH/AEP	Clotrimazole	21000121009	1
Caesar & Loretz GmbH/AHD	Clotrimazole	18147211	1
Caesar & Loretz GmbH/AHD	Clotrimazole	21000121010	1
Caesar & Loretz GmbH/AHD	Clotrimazole	21004117004	1
Caesar & Loretz GmbH...	Clotrimazole	21000121009	1
Caesar & Loretz GmbH...	Clotrimazole	19016105	1
Caesar & Loretz GmbH...	Clotrimazole	19016106	1
Caesar & Loretz GmbH...	Clotrimazole	20003904005	1
Caesar & Loretz GmbH...	Clotrimazole	21000123008	1
Caesar & Loretz GmbH/GEHE	Clotrimazole	18147211	1
Caesar & Loretz GmbH/Gehe	Clotrimazole	19016204	1
Caesar & Loretz GmbH/Gehe	Clotrimazole	20000092007	1
Caesar & Loretz GmbH/Gehe	Clotrimazole	20000094002	7
Caesar & Loretz GmbH/GEHE	Clotrimazole	20000094004	1
Caesar & Loretz GmbH/Gehe	Clotrimazole	21000121006	2
Caesar & Loretz GmbH/Gehe	Clotrimazole	21000123011	1
Caesar & Loretz GmbH/Gehe	Clotrimazole	21004117005	1
Caesar & Loretz GmbH...	Clotrimazole	20000092006	1
Caesar & Loretz GmbH...	Clotrimazole	21000121013	1
Caesar & Loretz GmbH...	Clotrimazole	21004116001	1
Caesar & Loretz GmbH...	Clotrimazole	19016105	1
Caesar & Loretz GmbH...	Clotrimazole	19016203	1
Caesar & Loretz GmbH...	Clotrimazole	20000094004	1
Caesar & Loretz GmbH...	Clotrimazole	20003904004	1
Caesar & Loretz GmbH...	Clotrimazole	21000121003	1
Caesar & Loretz GmbH...	Clotrimazole	19016206	1
Caesar & Loretz GmbH...	Clotrimazole	20003904003	1
Caesar & Loretz GmbH...	Clotrimazole	21000121010	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Clotrimazole	21000123011	1
Caesar & Loretz GmbH/K	Clotrimazole	20003904004	1
Caesar & Loretz GmbH...	Clotrimazole	20000094004	1
Caesar & Loretz GmbH...	Clotrimazole	21000121006	1
Caesar & Loretz GmbH...	Clotrimazole	18147102	1
Caesar & Loretz GmbH...	Clotrimazole	20000094002	1
Caesar & Loretz GmbH...	Clotrimazole	20000094005	1
Caesar & Loretz GmbH...	Clotrimazole	20000094008	1
Caesar & Loretz GmbH...	Clotrimazole	21000123006	1
Caesar & Loretz GmbH...	Clotrimazole	21000121006	1
Caesar & Loretz GmbH/Pho	Clotrimazole	21000121004	1
Caesar & Loretz GmbH...	Clotrimazole	21000121002	1
Caesar & Loretz GmbH...	Clotrimazole	21000123008	1
Caesar & Loretz GmbH...	Clotrimazole	21004116001	1
Caesar & Loretz GmbH...	Clotrimazole	21004116003	1
Caesar & Loretz GmbH...	Clotrimazole	21004117022	1
Caesar & Loretz GmbH...	Clotrimazole	20000094004	1
Caesar & Loretz GmbH...	Clotrimazole	21000121004	1
Caesar & Loretz GmbH...	Clotrimazole	21000121009	1
Caesar & Loretz GmbH...	Clotrimazole	21000121013	1
Caesar & Loretz GmbH...	Clotrimazole	21000123006	2
Caesar & Loretz GmbH...	Clotrimazole	21000123010	2
Caesar & Loretz GmbH...	Clotrimazole	20003904005	1
Caesar & Loretz GmbH...	Clotrimazole	21000121009	1
Caesar & Loretz GmbH...	Clotrimazole	19016119	2
Caesar & Loretz GmbH...	Clotrimazole	19016203	1
Caesar & Loretz GmbH...	Clotrimazole	19016204	1
Caesar & Loretz GmbH...	Clotrimazole	20000092005	1
Caesar & Loretz GmbH...	Clotrimazole	20000092007	1
Caesar & Loretz GmbH...	Clotrimazole	20000094004	1
Caesar & Loretz GmbH...	Clotrimazole	20000094006	2
Caesar & Loretz GmbH...	Clotrimazole	20003904004	1
Caesar & Loretz GmbH...	Clotrimazole	21000121002	2
Caesar & Loretz GmbH...	Clotrimazole	21000121003	2
Caesar & Loretz GmbH...	Clotrimazole	21000121004	1
Caesar & Loretz GmbH...	Clotrimazole	21000121008	1
Caesar & Loretz GmbH...	Clotrimazole	21000121009	2
Caesar & Loretz GmbH...	Clotrimazole	21000121010	1
Caesar & Loretz GmbH...	Clotrimazole	AP210225-03	1
Caesar & Loretz GmbH...	Clotrimazole	AP210622-01	1
Caesar & Loretz GmbH	Clotrimazole	16J07B02344817	1
Caesar & Loretz GmbH	Clotrimazole	17111604	1
Caesar & Loretz GmbH	Clotrimazole	17360204	3
Caesar & Loretz GmbH	Clotrimazole	17A19-B04	1
Caesar & Loretz GmbH	Clotrimazole	18147103	1
Caesar & Loretz GmbH	Clotrimazole	18147203	1
Caesar & Loretz GmbH	Clotrimazole	18147210	13
Caesar & Loretz GmbH	Clotrimazole	18147211	5
Caesar & Loretz GmbH	Clotrimazole	18147212	2
Caesar & Loretz GmbH	Clotrimazole	18147216	2
Caesar & Loretz GmbH	Clotrimazole	18147217	2
Caesar & Loretz GmbH	Clotrimazole	19016103	1
Caesar & Loretz GmbH	Clotrimazole	19016104	2
Caesar & Loretz GmbH	Clotrimazole	19016105	9
Caesar & Loretz GmbH	Clotrimazole	19016106	6
Caesar & Loretz GmbH	Clotrimazole	19016107	5
Caesar & Loretz GmbH	Clotrimazole	19016108	5
Caesar & Loretz GmbH	Clotrimazole	19016116	10
Caesar & Loretz GmbH	Clotrimazole	19016119	11
Caesar & Loretz GmbH	Clotrimazole	190162001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Clotrimazole	19016202	11
Caesar & Loretz GmbH	Clotrimazole	19016203	5
Caesar & Loretz GmbH	Clotrimazole	19016204	5
Caesar & Loretz GmbH	Clotrimazole	19016205	4
Caesar & Loretz GmbH	Clotrimazole	19016206	1
Caesar & Loretz GmbH	Clotrimazole	19016208	9
Caesar & Loretz GmbH	Clotrimazole	1902004-02	1
Caesar & Loretz GmbH	Clotrimazole	19076708	3
Caesar & Loretz GmbH	Clotrimazole	20000092002	7
Caesar & Loretz GmbH	Clotrimazole	20000092005	3
Caesar & Loretz GmbH	Clotrimazole	20000092006	14
Caesar & Loretz GmbH	Clotrimazole	20000092007	8
Caesar & Loretz GmbH	Clotrimazole	20000094002	2
Caesar & Loretz GmbH	Clotrimazole	20000094003	1
Caesar & Loretz GmbH	Clotrimazole	20000094004	8
Caesar & Loretz GmbH	Clotrimazole	20000094005	13
Caesar & Loretz GmbH	Clotrimazole	20000094006	13
Caesar & Loretz GmbH	Clotrimazole	20000094007	1
Caesar & Loretz GmbH	Clotrimazole	20000094008	9
Caesar & Loretz GmbH	Clotrimazole	20000094012	1
Caesar & Loretz GmbH	Clotrimazole	2000094004	2
Caesar & Loretz GmbH	Clotrimazole	2000094006	1
Caesar & Loretz GmbH	Clotrimazole	20003904002	2
Caesar & Loretz GmbH	Clotrimazole	20003904003	1
Caesar & Loretz GmbH	Clotrimazole	20003904004	13
Caesar & Loretz GmbH	Clotrimazole	20003904005	10
Caesar & Loretz GmbH	Clotrimazole	20003904008	2
Caesar & Loretz GmbH	Clotrimazole	21000121002	8
Caesar & Loretz GmbH	Clotrimazole	21000121003	11
Caesar & Loretz GmbH	Clotrimazole	21000121004	15
Caesar & Loretz GmbH	Clotrimazole	21000121005	1
Caesar & Loretz GmbH	Clotrimazole	21000121006	22
Caesar & Loretz GmbH	Clotrimazole	21000121008	2
Caesar & Loretz GmbH	Clotrimazole	21000121009	12
CAESAR & LORETZ GMBH	Clotrimazole	21000121009	1
Caesar & Loretz GmbH	Clotrimazole	21000121010	12
Caesar & Loretz GmbH	Clotrimazole	21000121013	9
Caesar & Loretz GmbH	Clotrimazole	21000123003	1
Caesar & Loretz GmbH	Clotrimazole	21000123006	15
Caesar & Loretz GmbH	Clotrimazole	21000123008	7
Caesar & Loretz GmbH	Clotrimazole	21000123010	2
Caesar & Loretz GmbH	Clotrimazole	21000123011	7
Caesar & Loretz GmbH	Clotrimazole	21004116001	13
Caesar & Loretz GmbH	Clotrimazole	21004116003	1
Caesar & Loretz GmbH	Clotrimazole	21004116005	2
Caesar & Loretz GmbH	Clotrimazole	21004116007	4
Caesar & Loretz GmbH	Clotrimazole	21004116014	5
Caesar & Loretz GmbH	Clotrimazole	21004117001	1
Caesar & Loretz GmbH	Clotrimazole	21004117003	1
Caesar & Loretz GmbH	Clotrimazole	21004117004	8
Caesar & Loretz GmbH	Clotrimazole	21004117005	10
Caesar & Loretz GmbH	Clotrimazole	21004117007	13
Caesar & Loretz GmbH	Clotrimazole	21004117011	3
Caesar & Loretz GmbH	Clotrimazole	21004117013	1
Caesar & Loretz GmbH	Clotrimazole	21004117016	2
Caesar & Loretz GmbH	Clotrimazole	21004117017	3
Caesar & Loretz GmbH	Clotrimazole	21004117018	2
Caesar & Loretz GmbH	Clotrimazole	21004117022	2
Caesar & Loretz GmbH	Clotrimazole	21I24-B11-213292	1
Caesar & Loretz GmbH...	Clotrimazole	20000092006	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Clotrimazole	20000094006	1
Caesar & Loretz Hild...	Clotrimazole	20003904003	1
Caesar & Loretz Hilden	Clotrimazole	18147211	1
Caesar & Loretz Hilden	Clotrimazole	19016204	1
Caesar & Loretz Hilden	Clotrimazole	20000094004	1
Caesar & Loretz/Geil...	Clotrimazole	18147203	1
Caesar & Loretz/Geil...	Clotrimazole	20000092005	1
Caesar & Loretz/Geil...	Clotrimazole	21000121002	2
Caesar & Loretz/Noweda	Clotrimazole	20000094002	1
Caesar & Loretz/Noweda	Clotrimazole	20000094005	1
Caesar & Loretz/Sanacorp	Clotrimazole	18147210	1
Caesar & Loretz	Clotrimazole	16234504	1
Caesar & Loretz	Clotrimazole	H20160502	1
Caesar u Loretz	Clotrimazole	15395613	1
Caesar u Loretz	Clotrimazole	16234501	1
Caesar&Lorenz / Gehe	Clotrimazole	19016199	1
Caesar&Lorenz	Clotrimazole	21000121002	1
Caesar&Loretz GmbH,1...	Clotrimazole	16234509	1
caesar&loretz GmbH,P...	Clotrimazole	15395614	1
Caesar&Loretz GmbH/ ...	Clotrimazole	16234522	1
Caesar&Loretz GmbH/Anzag	Clotrimazole	13184111	1
Caesar&Loretz GmbH/Anzag	Clotrimazole	14337807	1
Caesar&Loretz GmbH	Clotrimazole	14337814	1
Caesar&loretz,Phoenix	Clotrimazole	14144912	1
Caesar&LoretzGmbH, P...	Clotrimazole	18147212	1
Caesar/Gehe	Clotrimazole	20000092006	2
Caesar/Lorenz	Clotrimazole	12320814	1
Caesar/Lorenz	Clotrimazole	13224201	3
Caleo	Clotrimazole	15395610	1
CALO	Clotrimazole	17360204	1
Cealo/ Anzag	Clotrimazole	1703028-01	2
Cealo/GEHE	Clotrimazole	18147101	2
Cealo/Phoenix	Clotrimazole	19016106	1
Cealo/Sanacorp	Clotrimazole	1902004-03	1
Cealo	Clotrimazole	15395610	1
Cealo	Clotrimazole	17111612	1
Cealo	Clotrimazole	18147210	1
Delta	Clotrimazole	1607046-01	1
Dr. Wolff	Clotrimazole	1409027-04	2
E Plus	Clotrimazole	1703028-02	1
E Plus	Clotrimazole	1808028-01	2
EuRho / Phoenix	Clotrimazole	1703028-01	1
EuRho / Phoenix	Clotrimazole	2103024-02	4
EuRho / Phönix	Clotrimazole	2103024-01	1
EuRho /Gehe	Clotrimazole	1409027-02	1
EuRho AHC	Clotrimazole	1306036-01	1
EuRho Noweda	Clotrimazole	2007033-02	1
EuRho Noweda	Clotrimazole	2103024-01	1
EuRho/ Anzag	Clotrimazole	220629(2103024-01)	1
EuRho/ Fiebig	Clotrimazole	2007033-01	1
EuRho/ Phoenix	Clotrimazole	160704602	1
EuRho/ Phönix	Clotrimazole	1703028-02	1
EuRho/Gehe	Clotrimazole	2007033-01	1
EuRho/Gehe	Clotrimazole	2103024-01	1
EuRho/Kehr	Clotrimazole	1703028-02	1
EuRho/Noweda	Clotrimazole	2103024-02	1
EuRho/Phoenix	Clotrimazole	1210039-02	1
EuRho/Phoenix	Clotrimazole	1409027-01	1
EuRho/Phoenix	Clotrimazole	2007033-01	2
EuRho/Phoenix	Clotrimazole	2007033-03	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho/Phönix	Clotrimazole	1210039-2	1
EuRho/Phönix	Clotrimazole	1808028-01	1
Eurho/Phönix	Clotrimazole	200703302	1
EuRho/Sanacorp	Clotrimazole	16234522	1
EuRho	Clotrimazole	1108053-02	1
EuRho	Clotrimazole	1203040-02	2
EuRho	Clotrimazole	1203040-03	1
EuRho	Clotrimazole	1210039-02	2
EuRho	Clotrimazole	1306036-01	2
eurho	Clotrimazole	1309034-01	1
eurho	Clotrimazole	1309034-02	2
EuRho	Clotrimazole	1309034-02	1
EuRho	Clotrimazole	1409027-01	2
EuRho	Clotrimazole	1703028-01	2
Eurho	Clotrimazole	1703028-02	2
EuRho	Clotrimazole	18080028-01	1
EuRho	Clotrimazole	1808028-01	1
EuRho	Clotrimazole	1902004-01	5
EuRho	Clotrimazole	1902004-02	3
EuRho	Clotrimazole	1902204-01	1
EuRho	Clotrimazole	2007033-01	2
EuRho	Clotrimazole	2007033-02	1
EuRho	Clotrimazole	2103024-01	2
EuRhoNoweda	Clotrimazole	2103024-01	1
EuRhoPh/Ph	Clotrimazole	1902004-02	2
EuRhoPh/Ph	Clotrimazole	2007033-0130	1
Euro /BAUMANN	Clotrimazole	2007033-01	1
Euro Gehe	Clotrimazole	1808028-01	1
Euro OCT Pharma/ Sanacorp	Clotrimazole	1409027-04	1
Euro OT/Gehe	Clotrimazole	1409027-03	2
Euro OTC	Clotrimazole		6
Euro OTC	Clotrimazole	1008028	1
Euro OTC	Clotrimazole	1105014-01	1
Euro OTC	Clotrimazole	110501402	1
Euro OTC	Clotrimazole	1105014-02	1
Euro OTC	Clotrimazole	1108053-01	1
Euro OTC	Clotrimazole	1108053-02	2
Euro OTC	Clotrimazole	11808028-01	1
Euro OTC	Clotrimazole	1202004-03	1
Euro OTC	Clotrimazole	1203040	1
Euro OTC	Clotrimazole	1203040-01	1
Euro OTC	Clotrimazole	120304002	1
Euro OTC	Clotrimazole	1203040-02	8
Euro OTC	Clotrimazole	1203040-03	9
Euro OTC	Clotrimazole	12082013C	1
Euro OTC	Clotrimazole	1209211276	1
Euro OTC	Clotrimazole	121003901	3
Euro OTC	Clotrimazole	1210039-01	24
Euro OTC	Clotrimazole	1210039-02	22
Euro OTC	Clotrimazole	1306036	1
Euro OTC	Clotrimazole	130603601	3
Euro OTC	Clotrimazole	1306036-01	39
Euro OTC	Clotrimazole	1306306-01	1
Euro OTC	Clotrimazole	130636-01	2
Euro OTC	Clotrimazole	1309034	1
Euro OTC	Clotrimazole	130903401	5
Euro OTC	Clotrimazole	1309034-01	21
Euro OTC	Clotrimazole	130903402	1
Euro OTC	Clotrimazole	1309034-02	21
Euro OTC	Clotrimazole	1309054-02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Clotrimazole	1314Q1276	1
Euro OTC	Clotrimazole	13418014	1
Euro OTC	Clotrimazole	1409027	6
Euro OTC	Clotrimazole	1409027_03	1
Euro OTC	Clotrimazole	140902701	1
Euro OTC	Clotrimazole	1409027-01	29
Euro OTC	Clotrimazole	140902702	3
Euro OTC	Clotrimazole	1409027-02	44
Euro OTC	Clotrimazole	1409027-02Mg10g	1
Euro OTC	Clotrimazole	1409027-03	22
Euro OTC	Clotrimazole	1409027-04	30
Euro OTC	Clotrimazole	140927-01	1
Euro OTC	Clotrimazole	140927-02	1
Euro OTC	Clotrimazole	14144914	1
Euro OTC	Clotrimazole	14C04-B31-291660	1
Euro OTC	Clotrimazole	150003-01	1
Euro OTC	Clotrimazole	150003-02	1
Euro OTC	Clotrimazole	15010003-01	1
Euro OTC	Clotrimazole	15042014C	1
Euro OTC	Clotrimazole	15072014A	1
Euro OTC	Clotrimazole	151000	1
Euro OTC	Clotrimazole	151000-01	1
Euro OTC	Clotrimazole	1510003_01	1
Euro OTC	Clotrimazole	151000301	1
Euro OTC	Clotrimazole	1510003-01	57
Euro OTC	Clotrimazole	1510003-02	24
Euro OTC	Clotrimazole	151003-01	1
Euro OTC	Clotrimazole	1605003C	1
Euro OTC	Clotrimazole	1607045-01	1
Euro OTC	Clotrimazole	1607046	1
Euro OTC	Clotrimazole	1607046-0	1
Euro OTC	Clotrimazole	160704601	5
Euro OTC	Clotrimazole	1607046-01	71
Euro OTC	Clotrimazole	160704602	2
Euro OTC	Clotrimazole	1607046-02	40
Euro OTC	Clotrimazole	1607064-01	1
Euro OTC	Clotrimazole	16074046-01	1
Euro OTC	Clotrimazole	160802801	1
Euro OTC	Clotrimazole	1609046-01	1
Euro OTC	Clotrimazole	16234504	1
Euro OTC	Clotrimazole	16234505	1
Euro OTC	Clotrimazole	16234511	1
Euro OTC	Clotrimazole	16B11-B04-320088	1
Euro OTC	Clotrimazole	16J07-B02-341842	1
Euro OTC	Clotrimazole	170028-01	1
Euro OTC	Clotrimazole	1703025-03	1
Euro OTC	Clotrimazole	1703028	5
Euro OTC	Clotrimazole	1703028/03	1
Euro OTC	Clotrimazole	170302801	7
Euro OTC	Clotrimazole	1703028-01	119
Euro OTC	Clotrimazole	170302801-01	1
Euro OTC	Clotrimazole	170302802	1
Euro OTC	Clotrimazole	1703028-02	73
Euro OTC	Clotrimazole	1703028-02	1
Euro OTC	Clotrimazole	170302803	2
Euro OTC	Clotrimazole	1703028-03	62
Euro OTC	Clotrimazole	17053183	1
Euro OTC	Clotrimazole	170615C/1703028-01	1
Euro OTC	Clotrimazole	17111606	1
Euro OTC	Clotrimazole	17360201	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Clotrimazole	17A021	1
Euro OTC	Clotrimazole	17J25B06347476	1
Euro OTC	Clotrimazole	180002801	1
Euro OTC	Clotrimazole	180028-01	1
Euro OTC	Clotrimazole	1808018-01	1
Euro OTC	Clotrimazole	1808025-01	1
Euro OTC	Clotrimazole	1808028	4
Euro OTC	Clotrimazole	1808028_01	1
Euro OTC	Clotrimazole	1808028_02	1
Euro OTC	Clotrimazole	180802801	5
Euro OTC	Clotrimazole	1808028-01	129
Euro OTC	Clotrimazole	180802802	1
Euro OTC	Clotrimazole	1808028-02	79
Euro OTC	Clotrimazole	1808828-01	1
Euro OTC	Clotrimazole	18147211	1
Euro OTC	Clotrimazole	1828028-01	1
Euro OTC	Clotrimazole	19016108	1
Euro OTC	Clotrimazole	1902001-01	1
Euro OTC	Clotrimazole	1902004	2
Euro OTC	Clotrimazole	1902004_01	1
Euro OTC	Clotrimazole	190200401	7
Euro OTC	Clotrimazole	1902004-01	172
Euro OTC	Clotrimazole	1902004-01HZC14218	1
Euro OTC	Clotrimazole	190200402	1
Euro OTC	Clotrimazole	1902004-02	82
Euro OTC	Clotrimazole	190200403	2
Euro OTC	Clotrimazole	1902004-03	58
Euro OTC	Clotrimazole	190202004-02	1
Euro OTC	Clotrimazole	190204-01	2
Euro OTC	Clotrimazole	190204-03	1
Euro OTC	Clotrimazole	19022004-01	1
Euro OTC	Clotrimazole	19024004-01	1
Euro OTC	Clotrimazole	1904004-02	1
Euro OTC	Clotrimazole	192004-01	2
Euro OTC	Clotrimazole	20007033-01	1
Euro OTC	Clotrimazole	2007003-01	1
Euro OTC	Clotrimazole	200703-02	1
Euro OTC	Clotrimazole	2007033	1
Euro OTC	Clotrimazole	2007033_01	1
Euro OTC	Clotrimazole	200703301	5
Euro OTC	Clotrimazole	2007033-01	135
Euro OTC	Clotrimazole	2007033-02	70
Euro OTC	Clotrimazole	2007033-03	10
Euro OTC	Clotrimazole	2007033-1	1
Euro OTC	Clotrimazole	200733-02	1
Euro OTC	Clotrimazole	20130512	1
Euro OTC	Clotrimazole	20160801	5
Euro OTC	Clotrimazole	203024-02	1
Euro OTC	Clotrimazole	206718	1
Euro OTC	Clotrimazole	2103024	2
Euro OTC	Clotrimazole	2103024_02	1
Euro OTC	Clotrimazole	210302401	2
Euro OTC	Clotrimazole	2103024-01	85
Euro OTC	Clotrimazole	210302402	2
Euro OTC	Clotrimazole	2103024-02	46
Euro OTC	Clotrimazole	2103024-03	3
Euro OTC	Clotrimazole	2103024-04	1
Euro OTC	Clotrimazole	2103025-01	1
Euro OTC	Clotrimazole	21052015B	1
Euro OTC	Clotrimazole	21122013A	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Clotrimazole	213024-02	1
Euro OTC	Clotrimazole	220425D	1
Euro OTC	Clotrimazole	22091806	1
Euro OTC	Clotrimazole	22122014B	1
Euro OTC	Clotrimazole	2214A-01276	1
Euro OTC	Clotrimazole	230105501	3
Euro OTC	Clotrimazole	2301055-01	3
Euro OTC	Clotrimazole	23121408	1
Euro OTC	Clotrimazole	2313M01276	1
Euro OTC	Clotrimazole	2785	1
Euro OTC	Clotrimazole	2881	1
Euro OTC	Clotrimazole	30011402	1
Euro OTC	Clotrimazole	30062002	1
Euro OTC	Clotrimazole	3118A-01276	1
Euro OTC	Clotrimazole	3912E-01276	1
Euro OTC	Clotrimazole	40714/05	1
Euro OTC	Clotrimazole	41(1808028-01)	1
Euro OTC	Clotrimazole	4216M01276	1
Euro OTC	Clotrimazole	4216M-01276	2
Euro OTC	Clotrimazole	6051501	1
Euro OTC	Clotrimazole	700135	2
Euro OTC	Clotrimazole	H20160502	1
Euro OTC	Clotrimazole	HCZ00720	1
Euro OTC	Clotrimazole	HCZ06718	3
Euro OTC	Clotrimazole	HCZ07720	3
Euro OTC	Clotrimazole	HCZ14218	4
Euro OTC	Clotrimazole	HCZ20120	2
euro//Noweda	Clotrimazole	1808028-01	1
EUro/AHD	Clotrimazole	1210039-01	2
Euro/Gehe	Clotrimazole	1607046-02	1
Euro/Gehe	Clotrimazole	1703028-03	1
Euro/Gehe	Clotrimazole	18A18-B05-350778	1
Euro/Noweda	Clotrimazole	1510003-02	1
EURO/Noweda	Clotrimazole	190200401	1
Euro/Phönix	Clotrimazole	1510003-02	1
Euro/Phönix	Clotrimazole	1808028-01	1
Euro/Phönix	Clotrimazole	1902004-01	2
Euro/Sanacorp	Clotrimazole	1703028-02	1
Euro/Sanacorp	Clotrimazole	1808028-01	2
Euro	Clotrimazole	1510003-01	2
Euro	Clotrimazole	160704601	1
EuRoh/ Gehe	Clotrimazole	1808028-01	2
Euroo / Phönix	Clotrimazole	1409027-02	3
Europ Ots Pharma	Clotrimazole	13184105	1
Europharm/Otto	Clotrimazole	1203040-01	1
Europharm/Otto	Clotrimazole	1203040-02	1
europharma	Clotrimazole	1306036-01	1
EuroTOC / Noweda	Clotrimazole	1409027-03	1
Faggron	Clotrimazole	21/24-B11-213293	2
Fagron	Clotrimazole		5
Fagron	Clotrimazole	10G10B06-352427	1
Fagron	Clotrimazole	11A05-N14	2
Fagron	Clotrimazole	11E17-N10	2
Fagron	Clotrimazole	11F30-N14	2
Fagron	Clotrimazole	11G15-N10	1
Fagron	Clotrimazole	11K21-N19	1
Fagron	Clotrimazole	11L12-N10	5
Fagron	Clotrimazole	12/21-N01	5
Fagron	Clotrimazole	12/21-N04	3
Fagron	Clotrimazole	1210039-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clotrimazole	1221n04	1
Fagron	Clotrimazole	1221N04	1
Fagron	Clotrimazole	12721-N01	1
Fagron	Clotrimazole	12a05-n10	1
Fagron	Clotrimazole	12A05-N10	2
Fagron	Clotrimazole	12B27-N05	3
Fagron	Clotrimazole	12e02-N12	1
Fagron	Clotrimazole	12E02-N12	9
Fagron	Clotrimazole	12E30-N02	1
Fagron	Clotrimazole	12E30-N07	11
Fagron	Clotrimazole	12F02-N12	1
Fagron	Clotrimazole	12I16-N04	1
Fagron	Clotrimazole	12I21-N01	7
Fagron	Clotrimazole	12I21N04	1
Fagron	Clotrimazole	12I21-N04	7
Fagron	Clotrimazole	12K15-N01	1
Fagron	Clotrimazole	12l21-N04	2
Fagron	Clotrimazole	1309034-01	3
Fagron	Clotrimazole	13224201	1
Fagron	Clotrimazole	13C25-N10	9
Fagron	Clotrimazole	1409027-02	1
Fagron	Clotrimazole	14223201	1
Fagron	Clotrimazole	14337801	1
Fagron	Clotrimazole	14337818	1
Fagron	Clotrimazole	14337827	1
Fagron	Clotrimazole	14B05-B35	2
Fagron	Clotrimazole	14B05-B35-293542	3
Fagron	Clotrimazole	14B05-B35-293543	2
Fagron	Clotrimazole	14b05-b35-293544	1
Fagron	Clotrimazole	14B05-B35-293544	6
Fagron	Clotrimazole	14B05-B35-294932	1
Fagron	Clotrimazole	14b05-b35-294935	1
Fagron	Clotrimazole	14B05B35294935	1
Fagron	Clotrimazole	14B05-B35-294935	4
Fagron	Clotrimazole	14b05-b35-299941	1
Fagron	Clotrimazole	14B05-B35-299941	2
Fagron	Clotrimazole	14B05-B35-299944	3
Fagron	Clotrimazole	14B05-B36	7
Fagron	Clotrimazole	14B05B36291165	1
Fagron	Clotrimazole	14B05-B36-291165	2
Fagron	Clotrimazole	14b05b36291166	1
Fagron	Clotrimazole	14b05-b36-291166	1
Fagron	Clotrimazole	14B05-B36-291166	3
Fagron	Clotrimazole	14b05-B36-291167	1
Fagron	Clotrimazole	14B05B36291167	1
Fagron	Clotrimazole	14B05-B36-291167	5
Fagron	Clotrimazole	14B05-B36-291168	2
Fagron	Clotrimazole	14B05-B36-2991166	1
Fagron	Clotrimazole	14B06-B06	1
Fagron	Clotrimazole	14B06-B06-299942	1
Fagron	Clotrimazole	14B06-B06-299943	6
Fagron	Clotrimazole	14C04-B30	1
Fagron	Clotrimazole	14C04-B30-291656	10
Fagron	Clotrimazole	14C04-B30-291661	3
Fagron	Clotrimazole	14C04B31	1
Fagron	Clotrimazole	14C04-B31	8
Fagron	Clotrimazole	14C04-B312-299959	1
Fagron	Clotrimazole	14C04-B31-291660	4
Fagron	Clotrimazole	14C04-B31-294939	6
Fagron	Clotrimazole	14C04-B31-294940	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clotrimazole	14C04-B31-294951	1
Fagron	Clotrimazole	14C04-B31-294952	1
Fagron	Clotrimazole	14C04-B31-299954	7
Fagron	Clotrimazole	14C04-B31-299955	1
Fagron	Clotrimazole	14C04-B31-299959	2
Fagron	Clotrimazole	14C04-B31-299960	7
Fagron	Clotrimazole	14C04B32291657	1
Fagron	Clotrimazole	14C04-B32-291657	1
Fagron	Clotrimazole	14E26-B02	1
Fagron	Clotrimazole	1510003-01	1
Fagron	Clotrimazole	15G14-B05	4
Fagron	Clotrimazole	15G14-B05-311100	12
Fagron	Clotrimazole	15G14-B05-311101	1
Fagron	Clotrimazole	15G14-B05-311102	4
Fagron	Clotrimazole	15G14-B05-311103	13
Fagron	Clotrimazole	15G14-B05-316483	1
Fagron	Clotrimazole	15G14-B06	1
Fagron	Clotrimazole	15G14-B06-211057	1
Fagron	Clotrimazole	15G14-B06-31105	1
Fagron	Clotrimazole	15g14-b06-311054	1
Fagron	Clotrimazole	15G14B06311054	1
Fagron	Clotrimazole	15G14B06-311054	1
Fagron	Clotrimazole	15G14-B06-311054	4
Fagron	Clotrimazole	15G14-B06-311055	2
Fagron	Clotrimazole	15G14-B06-311056	2
Fagron	Clotrimazole	15G14-Bo5-311101	1
Fagron	Clotrimazole	160704602	1
Fagron	Clotrimazole	16234521	2
Fagron	Clotrimazole	16607-B02-333606	1
Fagron	Clotrimazole	16B09-B06	1
Fagron	Clotrimazole	16B09-B06-311506	4
Fagron	Clotrimazole	16B09-B06-311507	5
Fagron	Clotrimazole	16B09-B06-311785	2
Fagron	Clotrimazole	16B11B04	1
Fagron	Clotrimazole	16B11-B04	1
Fagron	Clotrimazole	16B11-B04-320088	6
Fagron	Clotrimazole	16B11-B04-322393	2
Fagron	Clotrimazole	16B11-B04-327611	6
Fagron	Clotrimazole	16BB11B04327611	1
Fagron	Clotrimazole	16E20-B10-317566	2
Fagron	Clotrimazole	16E20-B10-321597	2
Fagron	Clotrimazole	16E20-B10-321598	11
Fagron	Clotrimazole	16E20-B10-32197	1
Fagron	Clotrimazole	16E20-B10-324555	5
Fagron	Clotrimazole	16E20-B10-326010	3
Fagron	Clotrimazole	16E20-B10-327349	7
Fagron	Clotrimazole	16J07_B02	1
Fagron	Clotrimazole	16J07-B02	2
Fagron	Clotrimazole	16J07-B02-329385	4
Fagron	Clotrimazole	16J07-B02-329386	3
Fagron	Clotrimazole	16J07-B02-330216	7
Fagron	Clotrimazole	16J07-B02-330236	2
Fagron	Clotrimazole	16J07-B02-3335773	1
Fagron	Clotrimazole	16J07-B02-333606	3
Fagron	Clotrimazole	16J07-B02-335773	2
Fagron	Clotrimazole	16J07-B02-337573	3
Fagron	Clotrimazole	16J07-B02-338283	8
Fagron	Clotrimazole	16J07-B02-340511	2
Fagron	Clotrimazole	16j07-b02-340513	2
Fagron	Clotrimazole	16J07-B02-340513	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clotrimazole	16J07-B02-340513-201	1
Fagron	Clotrimazole	16J07B02341842	2
Fagron	Clotrimazole	16J07-B02-341842	1
Fagron	Clotrimazole	16J07-B02-344816	2
Fagron	Clotrimazole	16J07-B02-344817	4
Fagron	Clotrimazole	16J07-B02-344818	8
Fagron	Clotrimazole	16J07B02347864	1
Fagron	Clotrimazole	16J07-B02-347864	4
Fagron	Clotrimazole	16J23-F06-365713	1
Fagron	Clotrimazole	1703028-01	1
Fagron	Clotrimazole	1703028-03	1
Fagron	Clotrimazole	17111613	1
Fagron	Clotrimazole	17360201	1
Fagron	Clotrimazole	17A19-804-38560	2
Fagron	Clotrimazole	17A19-B04_332114	1
Fagron	Clotrimazole	17A19-B04-332097	2
Fagron	Clotrimazole	17A19-B04332114	1
Fagron	Clotrimazole	17A19-B04-332114	2
Fagron	Clotrimazole	17A19-B04-334768	4
Fagron	Clotrimazole	17A19-B04-336568	1
Fagron	Clotrimazole	17A19-B04-336581	1
Fagron	Clotrimazole	17A19-B04-338560	4
Fagron	Clotrimazole	17A19-B04-338577	4
Fagron	Clotrimazole	17A19-B04-340476	1
Fagron	Clotrimazole	17A19-B04-336568	1
Fagron	Clotrimazole	17A19-SB04-332097	1
Fagron	Clotrimazole	17J25-B06	3
Fagron	Clotrimazole	17J25-B06-345044	5
Fagron	Clotrimazole	17J25-B06-345045	2
Fagron	Clotrimazole	17J25-B06-345048	2
Fagron	Clotrimazole	17J25-B06-345049	1
Fagron	Clotrimazole	17J25-B06-345406	1
Fagron	Clotrimazole	17J25-B06-345407	3
Fagron	Clotrimazole	17J25-B06-347476	5
Fagron	Clotrimazole	17J25-B06-349130	2
Fagron	Clotrimazole	17j25-B06-349161	1
Fagron	Clotrimazole	17J25-B06-349161	6
Fagron	Clotrimazole	17J25-Bo6-345045	1
Fagron	Clotrimazole	17J25-BO6-349161	1
Fagron	Clotrimazole	18147101	1
Fagron	Clotrimazole	18147102	1
Fagron	Clotrimazole	18147217	1
Fagron	Clotrimazole	18610_B06	1
Fagron	Clotrimazole	18A18B05	1
Fagron	Clotrimazole	18A18-B05	1
Fagron	Clotrimazole	18A18-B05-344819	1
Fagron	Clotrimazole	18A18-B05-347865	10
Fagron	Clotrimazole	18a18-b05-348429	1
Fagron	Clotrimazole	18A18-B05348429	1
Fagron	Clotrimazole	18A18-B05-348429	4
Fagron	Clotrimazole	18A18-B05-349662	5
Fagron	Clotrimazole	18A18-B05-3496662	1
Fagron	Clotrimazole	18A18-B05-350778	9
Fagron	Clotrimazole	18A18-B05350780	1
Fagron	Clotrimazole	18A18-B05-350780	7
Fagron	Clotrimazole	18A18-B05-350781	2
Fagron	Clotrimazole	18A18B05352114	1
Fagron	Clotrimazole	18A18-B05-352114	4
Fagron	Clotrimazole	18a18-b05-352115	1
Fagron	Clotrimazole	18A18-B05-352115	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clotrimazole	18A18B05353892	1
Fagron	Clotrimazole	18A18-B05-353892	5
Fagron	Clotrimazole	18A18-B05-355041	2
Fagron	Clotrimazole	18A18-B05-355042	1
Fagron	Clotrimazole	18G10-B06	6
Fagron	Clotrimazole	18G10-B06-352425	4
Fagron	Clotrimazole	18G10-B06-352426	2
Fagron	Clotrimazole	18G10-B06-352427	5
Fagron	Clotrimazole	18G10-B06352708	1
Fagron	Clotrimazole	18G10-B06-352708	5
Fagron	Clotrimazole	18G10-b06-353348	1
Fagron	Clotrimazole	18G10-B06-353348	4
Fagron	Clotrimazole	18G10-B06-354620	1
Fagron	Clotrimazole	18G10-B06-355382	2
Fagron	Clotrimazole	18G10-B06-355401	3
Fagron	Clotrimazole	18G10-B06-358825	12
Fagron	Clotrimazole	19/23-F06-367383	1
Fagron	Clotrimazole	1902004-01	1
Fagron	Clotrimazole	19814-B01-363547	2
Fagron	Clotrimazole	19B01363546	1
Fagron	Clotrimazole	19B14-B01	8
Fagron	Clotrimazole	19B14-B01_363546	1
Fagron	Clotrimazole	19B14-B01-259532	1
Fagron	Clotrimazole	19B14-B01-359531	6
Fagron	Clotrimazole	19b14-b01-359532	1
Fagron	Clotrimazole	19B14-B01-359532	5
Fagron	Clotrimazole	19b14-b01-359537	1
Fagron	Clotrimazole	19B14B01359537	1
Fagron	Clotrimazole	19B14-B01-359537	6
Fagron	Clotrimazole	19B14-B01-359538	3
Fagron	Clotrimazole	19B14-B01-359539	11
Fagron	Clotrimazole	19B14-B01-359540	1
Fagron	Clotrimazole	19b14-b01-361607	1
Fagron	Clotrimazole	19B14-B01-361607	8
Fagron	Clotrimazole	19B14-B01-361608	3
Fagron	Clotrimazole	19B14B01361609	1
Fagron	Clotrimazole	19B14-B01-361609	5
Fagron	Clotrimazole	19B14-B01-361610	1
Fagron	Clotrimazole	19B14-B01-363546	21
Fagron	Clotrimazole	19B14-B01-363546/4320	1
Fagron	Clotrimazole	19B14-B01-363547	10
Fagron	Clotrimazole	19B14-B01-363557	13
Fagron	Clotrimazole	19B14-B1-363557	1
Fagron	Clotrimazole	19B14-BO1-363557	1
Fagron	Clotrimazole	19J23	1
Fagron	Clotrimazole	19j23-06-367383	1
Fagron	Clotrimazole	19J23-F06_365713	1
Fagron	Clotrimazole	19J23-F06_367381	3
Fagron	Clotrimazole	19J23-F06-365713	10
Fagron	Clotrimazole	19J23-F06-3673803	2
Fagron	Clotrimazole	19J23-F06-367381	5
Fagron	Clotrimazole	19J23F06-367382	1
Fagron	Clotrimazole	19J23-F06-367382	7
Fagron	Clotrimazole	19j23-f06-367383	3
Fagron	Clotrimazole	19J23-F06367383	1
Fagron	Clotrimazole	19J23-F06-367383	14
Fagron	Clotrimazole	19J23-FO6-367383	2
Fagron	Clotrimazole	1A1-B05-34765	1
Fagron	Clotrimazole	2007033-01	1
Fagron	Clotrimazole	20111018	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clotrimazole	20120603	3
Fagron	Clotrimazole	20151112-3	1
Fagron	Clotrimazole	20170427Ma9	1
Fagron	Clotrimazole	20171127Ma1	1
Fagron	Clotrimazole	20B27-F02	4
Fagron	Clotrimazole	20B27-F02_369401	1
Fagron	Clotrimazole	20B27-F02-0369401	1
Fagron	Clotrimazole	20B27-F02-369401	9
Fagron	Clotrimazole	20B27-F02-369402	4
Fagron	Clotrimazole	20b27f02369403	1
Fagron	Clotrimazole	20B27F02369403	2
Fagron	Clotrimazole	20B27-F02-369403	7
Fagron	Clotrimazole	20B27F02-370980	1
Fagron	Clotrimazole	20B27-F02-370980	1
Fagron	Clotrimazole	20H19-F01	1
Fagron	Clotrimazole	20H19-F01_37345	1
Fagron	Clotrimazole	20H19-F01-373455	3
Fagron	Clotrimazole	20H19-F01-373456	8
Fagron	Clotrimazole	20H26-F05	6
Fagron	Clotrimazole	20H26-F05-3737302	1
Fagron	Clotrimazole	20H26-F05-373732	3
Fagron	Clotrimazole	20H26-F05-373733	1
Fagron	Clotrimazole	20H26-F05-373736	4
Fagron	Clotrimazole	20H26-F05-373737	1
Fagron	Clotrimazole	20h26-f05-373738	1
Fagron	Clotrimazole	20H26F05373738	1
Fagron	Clotrimazole	20H26-F05-373738	3
Fagron	Clotrimazole	20H26-F05-373739	2
Fagron	Clotrimazole	20H26-F05-373740	2
Fagron	Clotrimazole	20H26-F06	1
Fagron	Clotrimazole	20H26-F06-373736	1
Fagron	Clotrimazole	20OH26-F05-373739	1
Fagron	Clotrimazole	21/24-B11-213289	1
Fagron	Clotrimazole	21/24-B11-213289Fag	1
Fagron	Clotrimazole	21/24-B11-218638	1
Fagron	Clotrimazole	21124-B11-218638	1
Fagron	Clotrimazole	2124-B11	1
Fagron	Clotrimazole	21B12-B10-216242	1
Fagron	Clotrimazole	21D22-B03-217092	8
Fagron	Clotrimazole	21D22-B03-217713	1
Fagron	Clotrimazole	21H13B14213291	1
Fagron	Clotrimazole	21H13-B14213291	1
Fagron	Clotrimazole	21H13-B14-213291	11
Fagron	Clotrimazole	21I24-B11-213289	2
Fagron	Clotrimazole	21I24B11213292	1
Fagron	Clotrimazole	21I24-B11-213292	7
Fagron	Clotrimazole	21I24-B11-213293	1
Fagron	Clotrimazole	21I24-B11-218638	4
Fagron	Clotrimazole	21l24-B11	1
Fagron	Clotrimazole	21l24-B11-218638	1
Fagron	Clotrimazole	22A21-B02-217360	4
Fagron	Clotrimazole	22A21-B02-217361	2
Fagron	Clotrimazole	22A21-B02-221730	2
Fagron	Clotrimazole	22A21-BO2-217360	1
Fagron	Clotrimazole	23D11-B01-228693	1
Fagron	Clotrimazole	2616A-01276	1
Fagron	Clotrimazole	2OB27-FO2-369402	1
Fagron	Clotrimazole	2OB27-FO2-369403	1
Fagron	Clotrimazole	3716Q-01276	1
Fagron	Clotrimazole	4812E-01276(NP)	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clotrimazole	6C16MU1	1
Fagron	Clotrimazole	700120-0003	2
Fagron	Clotrimazole	700135-0003	1
Fagron	Clotrimazole	8556777	1
Fagron	Clotrimazole	9041304	1
Fagron	Clotrimazole	A21130J001	2
Fagron	Clotrimazole	B01-3616009	1
Fagron	Clotrimazole	B01-3635406	1
Fagron	Clotrimazole	B01-3635507	1
Fagron	Clotrimazole	B11-213289	1
Fagron	Clotrimazole	C22H17CIN2	1
Fagron	Clotrimazole	CLT/1307/0065A	2
Fagron	Clotrimazole	CLT/150570016b	1
Fagron	Clotrimazole	CLT/160/00058	1
Fagron	Clotrimazole	CLT/1604/00227A	1
Fagron	Clotrimazole	CLT/1604/0027A	2
Fagron	Clotrimazole	CLT/1607/0060A	2
Fagron	Clotrimazole	CLT/1709/0067B	1
Fagron	Clotrimazole	CLT/1711/0077A	2
Fagron	Clotrimazole	CLT/1805/00468	2
Fagron	Clotrimazole	CLT/1805/0046B	2
Fagron	Clotrimazole	CLT/1805/0064B	3
Fagron	Clotrimazole	CLT/1901/0002A	5
Fagron	Clotrimazole	CLT/2001/0006A	1
Fagron	Clotrimazole	CLT-1805-0046B	1
Fagron	Clotrimazole	F01-3734506	2
Fagron	Clotrimazole	F0236940001	1
Fagron	Clotrimazole	F02-3694001	4
Fagron	Clotrimazole	F02-3694002	1
Fagron	Clotrimazole	F02-3709800	1
Fagron	Clotrimazole	F05-3737302	1
Fagron	Clotrimazole	F06-3657103	1
Fagron	Clotrimazole	F06-3673801	2
Fagron	Clotrimazole	F06-3673803	3
Fagron	Clotrimazole	HCZ11520	4
Fargon/ Phoenix	Clotrimazole	18G10-B06-358825	1
Fargon/Noweda	Clotrimazole	18G-10-B06-355401	1
Fargon/Noweda	Clotrimazole	19B14-B01-363557	1
Fargon/Phönix	Clotrimazole	18147103	1
Fargon	Clotrimazole	16234511	1
Fargon	Clotrimazole	17J25-B06-345406	1
Fargon	Clotrimazole	18A18-B05-350778	1
Fargon	Clotrimazole	18g10-b06-355401	1
Fargon	Clotrimazole	18G10-B06-355401	1
Fargon	Clotrimazole	19B14-B01-363547	1
Fargon	Clotrimazole	20B27-F02-369403	1
Fargron / Noweda	Clotrimazole	16E20-B10-324555	1
Fiebig 10.06.13 ek: 8,58EUR	Clotrimazole	12E30-N07	1
Fiebig	Clotrimazole	1607046-01	1
Fiebig	Clotrimazole	1607046-02	1
Fiebig	Clotrimazole	1703028	1
Fiebig	Clotrimazole	1703028-03	1
Fiebig	Clotrimazole	1808028-02	1
Fiebig	Clotrimazole	18147101	1
Fiebig	Clotrimazole	20000092006	1
Fiebig	Clotrimazole	20000094008	1
Finteler Apotheke	Clotrimazole	16234501	1
Finteler Apotheke	Clotrimazole	16234509	1
Fischar/Gehe	Clotrimazole	20111018	1
Fragon	Clotrimazole	19B14-B01-363557	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fragon	Clotrimazole	21H13-B14-218610	1
Fragron/noweda	Clotrimazole	17A19-B04	1
Fragron/noweda	Clotrimazole	CLT/1601/0005B	1
Gatt-Koller	Clotrimazole	1801870	1
Gatt-Koller	Clotrimazole	201714s9	1
Gehe amax	Clotrimazole	14B05-B35-294935	1
Gehe amax	Clotrimazole	1607046-02	1
Gehe amax	Clotrimazole	16J07-B02-330216	1
Gehe amax	Clotrimazole	17111608	1
Gehe amax	Clotrimazole	1808028-01	1
Gehe amax	Clotrimazole	19J23-F06-365713	1
Gehe amax	Clotrimazole	20000092005	1
Gehe	Clotrimazole	1108053-01	1
Gehe	Clotrimazole	11K21-N19	1
Gehe	Clotrimazole	12/21-N01	1
Gehe	Clotrimazole	121003902	1
Gehe	Clotrimazole	1306036-01	3
Gehe	Clotrimazole	1309034-01	1
Gehe	Clotrimazole	13184103	1
Gehe	Clotrimazole	13224216	1
Gehe	Clotrimazole	1409027-02	2
Gehe	Clotrimazole	14337815	2
Gehe	Clotrimazole	14337819	1
Gehe	Clotrimazole	14B05B35294935	1
Gehe	Clotrimazole	14B05-B35-294935	1
Gehe	Clotrimazole	14C04-B31-294952	1
Gehe	Clotrimazole	15G14-B05	1
GEHE	Clotrimazole	1607046-02	1
Gehe	Clotrimazole	16234505	1
Gehe	Clotrimazole	16234511	1
Gehe	Clotrimazole	16234513	1
GEHE	Clotrimazole	16234513	1
Gehe	Clotrimazole	16E20-B10-321598	2
GEHE	Clotrimazole	16J07-B02	1
Gehe	Clotrimazole	16j07-b02-330216	1
Gehe	Clotrimazole	16J07-B02-330216	1
Gehe	Clotrimazole	1703028-02	1
Gehe	Clotrimazole	17111603	1
Gehe	Clotrimazole	17111605	1
Gehe	Clotrimazole	17111616	1
Gehe	Clotrimazole	17360201	1
GEHE	Clotrimazole	17360202	1
GEHE	Clotrimazole	177111613	1
Gehe	Clotrimazole	17A19-B04	1
Gehe	Clotrimazole	17A19-B04-338560	1
Gehe	Clotrimazole	17J25-B06-0345044	1
Gehe	Clotrimazole	17J25-B06-345048	1
Gehe	Clotrimazole	17J25-B06-345407	1
Gehe	Clotrimazole	1808028-01	4
Gehe	Clotrimazole	1808028-02	1
Gehe	Clotrimazole	18147101	1
Gehe	Clotrimazole	18147103	1
GEHE	Clotrimazole	18147103	1
GEHE	Clotrimazole	18147210	2
Gehe	Clotrimazole	18A18-B05-350778	1
Gehe	Clotrimazole	18G10-B06	2
Gehe	Clotrimazole	18G10-B06-0046B	1
Gehe	Clotrimazole	18G10-B06-358825	1
Gehe	Clotrimazole	19016106	1
Gehe	Clotrimazole	19016108	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Clotrimazole	19016116	1
Gehe	Clotrimazole	1902004-02	2
Gehe	Clotrimazole	1902004-03	2
Gehe	Clotrimazole	200000094004	1
gehe	Clotrimazole	20000092002	1
Gehe	Clotrimazole	20000092006	1
Gehe	Clotrimazole	20000094003	2
Gehe	Clotrimazole	20000094006	1
Gehe	Clotrimazole	2007033-02	1
Gehe	Clotrimazole	21000123006	2
Gehe	Clotrimazole	21004116005	1
Gehe	Clotrimazole	21004116007	2
Gehe	Clotrimazole	21004116013	1
Gehe	Clotrimazole	21004116014	3
gehe	Clotrimazole	21004116016	1
Gehe	Clotrimazole	21004117003	1
Gehe	Clotrimazole	21004117007	1
Gehe	Clotrimazole	21004117016	1
Gehe	Clotrimazole	21004117018	1
Gehe	Clotrimazole	2103021-01	1
Gehe	Clotrimazole	2103024-01	1
Gehe	Clotrimazole	22A21-B02-217361	1
GEHE	Clotrimazole	23001596002	1
Gehe	Clotrimazole	23001596008	2
Gehe	Clotrimazole	2301055-01	1
Gehe	Clotrimazole	CLT/1805/0046B	1
Gehe	Clotrimazole	HCZ14218	1
Geilenkirchen	Clotrimazole	17360204	1
Geilenkirchen	Clotrimazole	20000094004	1
Guangzhou Hanpu Phar...	Clotrimazole	14337819	1
Guangzhou Hanpu Phar...	Clotrimazole	1409027-03	1
Guangzhou Hanpu Phar...	Clotrimazole	1510003-01	1
Guangzhou Hanpu Phar...	Clotrimazole	1510003-02	1
Guangzhou Hanpu Pharmac.	Clotrimazole	1703028-02	1
Halcycon Labs	Clotrimazole	19016104	1
Halcyon / Noweda	Clotrimazole	18147210	1
Halcyon Labs / Gehe ...	Clotrimazole	18147103	1
Halcyon Labs Pvt. Lt...	Clotrimazole	20000094006	1
Halcyon Labs Pvt.Ltd...	Clotrimazole	W8269	1
Halcyon Labs Pvt.Ltd...	Clotrimazole	18147101	1
Halcyon Labs Pvt	Clotrimazole	20003904004	1
Halcyon Labs/	Clotrimazole	19016105	1
Halcyon Labs	Clotrimazole	1808028-02	1
Halcyon Labs	Clotrimazole	20000094005	1
Halcyon/Link & Eccius	Clotrimazole	W8269	1
Halcyon/Noweda	Clotrimazole	20000094008	1
Halcyon/Noweda	Clotrimazole	HCZ14518	1
Halcyon/Noweda	Clotrimazole	HCZ14718	1
Halycon Labs / Fiebig	Clotrimazole	HCZ06718	1
Hedinger/Alliance H.	Clotrimazole	15395617	2
Hedinger/Gehe	Clotrimazole	1703028-02	1
Henry Lamotte oils GmbH	Clotrimazole	18147203	1
Jenne	Clotrimazole	18147103	1
Jenne	Clotrimazole	20000092006	1
JENNE	Clotrimazole	21004116007	1
Jenne	Clotrimazole	23001596009	2
Jenne	Clotrimazole	2301055-01	1
Kehr	Clotrimazole	1808028-01	1
Kehr	Clotrimazole	18g10-b06-3533348	1
Kehr	Clotrimazole	18g10-b06-353348	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Kehr	Clotrimazole	21004116013	1
Kehr	Clotrimazole	21004116014	1
Kehr	Clotrimazole	21004117022	1
Kehr	Clotrimazole	2103024-02	1
Kehr	Clotrimazole	2301055-01	2
Klenk	Clotrimazole	16B09-B06-311785	1
Klosterring	Clotrimazole	16234512	1
Klosterring	Clotrimazole	17111615	2
Klosterring	Clotrimazole	6234505	1
L12	Clotrimazole	16234512	1
L12	Clotrimazole	17111606	1
L12	Clotrimazole	17360204	1
Link &Eccius (Halcyo...	Clotrimazole	W8269	1
Maros Arznei GmbH	Clotrimazole	13184105	1
Martin Apo	Clotrimazole	31117/1	1
Midas	Clotrimazole	1703028-01	1
Midas	Clotrimazole	1703028-03	1
Midas	Clotrimazole	1808028-02	1
Mvda_15.01.2019	Clotrimazole	18147102	1
Nachprüfung	Clotrimazole	2082019-4	1
Noveda	Clotrimazole	20003904003	1
Noweda 06.11.2019	Clotrimazole	19016119	1
Noweda 07.07.2015	Clotrimazole	14144913	1
Noweda 17.7.2019	Clotrimazole	19016105	1
Noweda Fiebig 15.05....	Clotrimazole	20000092002	1
Noweda Taucha	Clotrimazole	19016206	1
Noweda/EuRho	Clotrimazole	2103024-01	1
Noweda/Fargon	Clotrimazole	17A19-B04-336568	1
Noweda	Clotrimazole	1203040-03	2
Noweda	Clotrimazole	13224201	1
Noweda	Clotrimazole	13224217	1
Noweda	Clotrimazole	1409027	1
Noweda	Clotrimazole	1409027-02	1
Noweda	Clotrimazole	14337801	1
Noweda	Clotrimazole	14337816	1
Noweda	Clotrimazole	1510003-01	2
Noweda	Clotrimazole	15G14-B05-316483	2
Noweda	Clotrimazole	16234511	3
Noweda	Clotrimazole	16234517	2
Noweda	Clotrimazole	16J07-B02-329386	1
Noweda	Clotrimazole	16j07-b02-341842	1
Noweda	Clotrimazole	1703028-01	1
Noweda	Clotrimazole	17111608	1
Noweda	Clotrimazole	17360201	1
Noweda	Clotrimazole	17360203	2
Noweda	Clotrimazole	17J25-B06-345044	1
Noweda	Clotrimazole	18147203	2
Noweda	Clotrimazole	18147211	1
Noweda	Clotrimazole	18147212	1
Noweda	Clotrimazole	18A18-B05	1
Noweda	Clotrimazole	18G10-B06	1
Noweda	Clotrimazole	18G10-B06-352425	1
Noweda	Clotrimazole	18G10-B06-358825	2
Noweda	Clotrimazole	19016104	1
Noweda	Clotrimazole	19016107	1
Noweda	Clotrimazole	19016202	2
Noweda	Clotrimazole	19016204	1
Noweda	Clotrimazole	19016208	1
Noweda	Clotrimazole	19020004-01	1
Noweda	Clotrimazole	1902004_01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Clotrimazole	1902004-02	1
Noweda	Clotrimazole	19B14-B01-359539	1
Noweda	Clotrimazole	20000094005	1
Noweda	Clotrimazole	2007033-01	1
Noweda	Clotrimazole	2007033-02	2
Noweda	Clotrimazole	20111115	1
Noweda	Clotrimazole	20H26-F05-373738	1
Noweda	Clotrimazole	20H26-F05-373739	4
Noweda	Clotrimazole	21000121002	1
Noweda	Clotrimazole	21000123008	1
Noweda	Clotrimazole	21000123011	1
Noweda	Clotrimazole	21004116013	1
Noweda	Clotrimazole	21004117001	1
Noweda	Clotrimazole	21004117018	2
Noweda	Clotrimazole	21004117019	2
Noweda	Clotrimazole	2103024-01	1
Noweda	Clotrimazole	2103024-03	1
Noweda	Clotrimazole	21H13-B14-213291	2
Noweda	Clotrimazole	22A21-B02-221730	1
Noweda	Clotrimazole	2301055-01	1
Oberlinden Apotheke	Clotrimazole	201401300378	2
p&m cosmetics/gehe	Clotrimazole	16J07-B02-335773	2
Phö/Dr.Wolff	Clotrimazole	19016108	1
Phoenix 23.10.14 5,50	Clotrimazole	1309034-02	1
Phoenix 24.04.2017	Clotrimazole	1607046-02	1
PHOENIX am 22.01.2014	Clotrimazole	1306036-01	1
Phoenix	Clotrimazole	12A05-N10	1
Phoenix	Clotrimazole	1309034-02	1
Phoenix	Clotrimazole	13224215	1
Phoenix	Clotrimazole	14337812	1
Phoenix	Clotrimazole	14c04b31	1
Phoenix	Clotrimazole	1607046-01	1
Phoenix	Clotrimazole	16234509	1
phoenix	Clotrimazole	16234512	1
Phoenix	Clotrimazole	16B11-B04-327611	1
Phoenix	Clotrimazole	17111601	1
Phoenix	Clotrimazole	17111603	1
Phoenix	Clotrimazole	18147102	1
Phoenix	Clotrimazole	1902004-01	1
Phoenix	Clotrimazole	1902004-02	2
Phoenix	Clotrimazole	191381012	1
Phoenix	Clotrimazole	20000092006	1
Phoenix	Clotrimazole	20000094003	1
Phoenix	Clotrimazole	20003904004	1
Phoenix	Clotrimazole	21000121002	1
phoenix	Clotrimazole	21000121004	3
Phoenix	Clotrimazole	21000121006	1
Phoenix	Clotrimazole	21004116014	1
Phoenix	Clotrimazole	21004117004	1
Phoenix	Clotrimazole	21004117016	1
Phoenix	Clotrimazole	21004117017	1
Phoenix	Clotrimazole	2103024-02	1
Phoenix	Clotrimazole	22A21-B02-217361	1
Phoenix	Clotrimazole	23001596002	1
Phoenix	Clotrimazole	2301055-01	1
Phoenix	Clotrimazole	3088	1
Phoenix	Clotrimazole	3237	1
Phoenix	Clotrimazole	79879	1
Phönix Gotha	Clotrimazole	14337811	1
Phönix Gotha	Clotrimazole	16J07-B02-344816	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix WE:23.10.17 ...	Clotrimazole	16234521	1
Phönix	Clotrimazole		1
phönix	Clotrimazole	11305513	1
Phönix	Clotrimazole	13C25-N10	1
Phönix	Clotrimazole	1409027-01	1
phönix	Clotrimazole	14337818	1
Phönix	Clotrimazole	15395618	1
Phönix	Clotrimazole	1607046-01	1
Phönix	Clotrimazole	16234505	1
phönix	Clotrimazole	16234512	1
phönix	Clotrimazole	16B11-B04-327611	1
Phönix	Clotrimazole	1703028-03	1
Phönix	Clotrimazole	17111603	1
Phönix	Clotrimazole	17111604	1
Phönix	Clotrimazole	17111608	2
Phönix	Clotrimazole	17360203	1
Phönix	Clotrimazole	18147103	1
Phönix	Clotrimazole	18147203	1
PHÖNIX	Clotrimazole	18147203	1
Phönix	Clotrimazole	18147212	1
Phönix	Clotrimazole	18G10-B06-354620	2
Phönix	Clotrimazole	19016104	1
Phönix	Clotrimazole	19016108	1
Phönix	Clotrimazole	19016116	1
Phönix	Clotrimazole	19016203	1
Phönix	Clotrimazole	19016205	1
Phönix	Clotrimazole	1902004-01	2
Phönix	Clotrimazole	1902004-02	1
Phönix	Clotrimazole	1902004-03	2
PHÖNIX	Clotrimazole	19b14b01363546	1
Phönix	Clotrimazole	20000092007	1
Phönix	Clotrimazole	2007033-01	1
PHÖNIX	Clotrimazole	200703301	1
Phönix	Clotrimazole	2007033-03	1
Phönix	Clotrimazole	200742407	1
Phönix	Clotrimazole	201033-01	1
Phönix	Clotrimazole	20160801	1
Phönix	Clotrimazole	21000121002	1
Phönix	Clotrimazole	21004116007	2
Phönix	Clotrimazole	21004116013	1
Phönix	Clotrimazole	21004116016	1
Phönix	Clotrimazole	21004117022	1
Phönix	Clotrimazole	2103024-01	1
Phönix	Clotrimazole	23001596002	2
Phönix	Clotrimazole	23001596003	2
Phönix	Clotrimazole	23003390001	1
Röntgen	Clotrimazole	1703028-01	5
Röntgen	Clotrimazole	1808028-01	3
Röntgen	Clotrimazole	1902004-03	1
Röntgen	Clotrimazole	2007033-02	1
Röntgen	Clotrimazole	2103024-01	1
Sanacorp/Caela	Clotrimazole	17111603	1
Sanacorp	Clotrimazole	105/AKD1	1
Sanacorp	Clotrimazole	109/AKD3	1
Sanacorp	Clotrimazole	109/AKD6	1
Sanacorp	Clotrimazole	1203040-03	1
Sanacorp	Clotrimazole	12159902	1
Sanacorp	Clotrimazole	1230805	1
Sanacorp	Clotrimazole	12320814	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Clotrimazole	13184105	1
Sanacorp	Clotrimazole	13224214	2
Sanacorp	Clotrimazole	13224219	1
Sanacorp	Clotrimazole	14144905	1
sanacorp	Clotrimazole	14144918	1
Sanacorp	Clotrimazole	14337817	1
Sanacorp	Clotrimazole	15g14-b05-311100	1
Sanacorp	Clotrimazole	16E20-B10-327349	1
Sanacorp	Clotrimazole	16J07-B02-330216	1
Sanacorp	Clotrimazole	16J07-B02-338283	1
Sanacorp	Clotrimazole	1703028-02	1
Sanacorp	Clotrimazole	170302803	1
Sanacorp	Clotrimazole	17360201	1
Sanacorp	Clotrimazole	17360203	1
Sanacorp	Clotrimazole	18147102	1
Sanacorp	Clotrimazole	18147210	2
Sanacorp	Clotrimazole	18147211	1
Sanacorp	Clotrimazole	18147212	1
Sanacorp	Clotrimazole	1882321	1
Sanacorp	Clotrimazole	18G10-B06	1
Sanacorp	Clotrimazole	19016116	1
Sanacorp	Clotrimazole	19016203	3
Sanacorp	Clotrimazole	19016208	2
Sanacorp	Clotrimazole	19B14-B01-359537	1
Sanacorp	Clotrimazole	20000094006	1
Sanacorp	Clotrimazole	20000094008	1
sanacorp	Clotrimazole	20003904004	1
Sanacorp	Clotrimazole	20003904005	1
Sanacorp	Clotrimazole	200703302	1
Sanacorp	Clotrimazole	20H19-F01	1
Sanacorp	Clotrimazole	20H26-F05	1
Sanacorp	Clotrimazole	21000121006	2
Sanacorp	Clotrimazole	21000123008	1
Sanacorp	Clotrimazole	21000123010	1
Sanacorp	Clotrimazole	21004116013	1
Sanacorp	Clotrimazole	21004116014	2
Sanacorp	Clotrimazole	21004116017	1
sanacorp	Clotrimazole	21004117005	1
Sanacorp	Clotrimazole	21D22-B03-217092	2
Sanacorp	Clotrimazole	21H13-B14-213291	1
Sanacorp	Clotrimazole	22A21-B02-221671	1
Sanacorp	Clotrimazole	23001596003	1
sanacorp	Clotrimazole	2301055-01	1
Sanacorp	Clotrimazole	APCLT/1703/0016CC	1
Sino Phyto	Clotrimazole	13224210	2
Stumpf	Clotrimazole	12159902	1
Vdl 14.07.14	Clotrimazole	13224225	1
VDL;11.06.15;27,90EUR	Clotrimazole	14337807	1
WE Phönix.01.12.2016...	Clotrimazole	15395618	1
wepa/Sanaco	Clotrimazole	14337819	1

- 229 124 spectra from 1515 *Apo-Ident* customers from a total of 48 342 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Clotrimazole* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Clotrimazole* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	540	0	152 422
Type B	0	640	0	201 444
Type C	0	6858	85	229 124

The substance/substance group *Clotrimazole* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8889 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0625 %)
Type C	100.0000 % (> 99.9007 %)	98.7757 % (> 98.7325 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20794	22229	6.09	60.32
21087	23791	9.03	62.60
21114	23791	8.80	59.16
21207	25649	7.34	54.96
21259	25649	10.25	57.55
21264	25656	4.66	55.46
21352	22229	8.41	59.45
21353	22229	8.88	59.06
22229	22229	0.00	63.00
23791	23791	0.00	57.61
25649	25649	0.00	52.59
25656	25656	0.00	53.46
26137	25656	25.97	47.16

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Colistin sulfate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20318-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Colistin sulfate; Colistin sulphate; Colistini sulfas

Special notes

When selecting the *Colistin sulfate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Colistin sulfate	10	10	14

Second-stage model

For differentiation of the substance/substance group *Colistin sulfate* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Colistin sulfate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	30.16	19.07
Bacitracin	37.51	13.73
Calcium pantothenate	73.77	37.92
⋮	⋮	⋮
Amphotericin B	>50	47.48
alpha-tocopheryl acetate dry concentrate	>50	53.69
Cyanocobalamin	>50	56.43
Riboflavin	>50	65.17
Selenium yeast	>50	65.82
Methylcobalamin	>50	67.50
Nystatin	>50	70.19
Gelatine, white	>50	73.76
Estradiol hemihydrate	>50	75.59
Estriol	>50	77.96
Triamcinolone	>50	87.83
Calcium glycerophosphate	>50	102.98
Carmellose sodium	>50	129.47
Hyoscine hydrobromide	>50	158.25
SyrSpend® SF Alka	>50	199.28
Tosylchloramide sodium	>50	202.04
Rice starch	>50	230.94
SyrSpend® SF pH4 neo (Maize starch)	>50	288.81
Oxalic acid	>50	315.11
Acacia, dried dispersion	>50	324.46
Corn starch	>50	326.55
SyrSpend® SF pH4	>50	402.15
Maltodextrin	>50	453.41
Potato starch	>50	463.39
Wheat starch	>50	469.46
Fructose	>50	552.70

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Colistin sulfate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Colistin sulfate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Colistin sulfate	APKB-CS-1602026C	22974	40	20160418
Audor Pharma	Colistin sulfate	APKB-CS-1602026C	23027	40	20160418
Euro OTC	Colistin sulfate	1406001-01	21619	60	1508600
Euro OTC	Colistin sulfate	1507044	21852	60	20150817*
Euro OTC	Colistin sulfate	1602021	22371	60	20160307*
Euro OTC	Colistin sulfate	1606008	22695	40	20160704*
Euro OTC	Colistin sulfate	2009035	25431	40	20200930*
Fagron	Colistin sulfate	13G05-N01	20915	40	20130719
Fagron	Colistin sulfate	13G05-N01	21209	40	20130719
Fagron	Colistin sulfate	14E02-B03	21346	40	1501654
Fagron	Colistin sulfate	16F03-B01-324216	22973	40	20160706
Fagron	Colistin sulfate	20F18-B04-201974	25667	50	20200706

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 550 spectra of 12 reference samples from the substance/substance group *Colistin sulfate*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.
- 152 412 spectra from a total of 2832 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 465 spectra of 13 reference samples from the substance/substance group *Colistin sulfate*.
- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Audor Pharma	Colistin sulfate	APKB-CS-1603034C	23026	40
Euro OTC	Colistin sulfate	1406002-01	21700	45
Euro OTC	Colistin sulfate	1709009	23616	40
Euro OTC	Colistin sulfate	1710041	23866	40
Euro OTC	Colistin sulfate	1905016	24769	40
Euro OTC	Colistin sulfate	1908007	24836	40
Euro OTC	Colistin sulfate	2001039	25087	40
Euro OTC	Colistin sulfate	2301012	26653	40
Fagron	Colistin sulfate	22B14-B10-219015	26182	40
Fagron	Colistin sulfate	23D12-B10-230780	27382	40
Euro OTC	Colistin sulfate	2301012	26653SI	20
Fagron	Colistin sulfate	22B14-B10-219015	26182SI	20
Fagron	Colistin sulfate	23D12-B10-230780	27382SI	20

- 201 619 spectra from a total of 4035 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 18 spectra from 8 *Apo-Ident* customers from 16 batches from the substance/substance group *Colistin sulfate*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Audor Pharma	Colistin sulfate	APKB-CS-1601026C	1
Audor Pharma	Colistin sulfate	APKB-CS-1603034C	2
Audor Pharma	Colistin sulfate	APKB-CS-1610012C	1
Caelo	Colistin sulfate	1602021-01	1
Euro OTC	Colistin sulfate	1507044-01	1
Fagron	Colistin sulfate	15E15-B01-315340	1
Fagron	Colistin sulfate	16F03-B01	1
Fagron	Colistin sulfate	16F03-B01_322758	1
Fagron	Colistin sulfate	16f03-b01-324216	1
Fagron	Colistin sulfate	16F03-B01-324216	1
Fagron	Colistin sulfate	16J03-B10-330367	1
Fagron	Colistin sulfate	17E09-B04-342085	1
Fagron	Colistin sulfate	17j24-b03-342638	1
Fagron	Colistin sulfate	20K06-B03-202435	2
Fagron	Colistin sulfate	21G20_B09213652	1
Fagron	Colistin sulfate	21G20-B08-215430	1

- 236 049 spectra from 1515 *Apo-Ident* customers from a total of 49 242 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Colistin sulfate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Colistin sulfate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	512	38	152 412
Type B	0	465	0	201 619
Type C	0	18	0	236 049

The substance/substance group *Colistin sulfate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	93.0909 % (> 92.5455 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.7097 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20915	21619	8.77	49.67
21209	21619	8.04	45.61
21346	21346	0.00	37.09
21619	21619	0.00	46.23
21852	21852	0.00	37.27
22371	22371	0.00	53.81
22695	22695	0.00	38.27
22973	21852	3.20	36.84
22974	21852	16.60	36.05
23027	21346	17.16	35.74
25431	25431	0.00	59.54
25667	22695	23.61	37.51

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cyanocobalamin / Methylcobalamin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10003566-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cyanocobalamin / Methylcobalamin; Cyanocobalamin; Cyanocobalaminum; Methylcobalamin

Special notes

When selecting the *Cyanocobalamin / Methylcobalamin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cyanocobalamin / Methylcobalamin	16	10	33

Second-stage model

For differentiation of the substance/substance group *Cyanocobalamin / Methylcobalamin* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cyanocobalamin / Methylcobalamin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Bacitracin	40.78	14.86
Polymyxin B sulfate	45.31	24.47
⋮	⋮	⋮
Colistin sulfate	>50	29.63
Amphotericin B	>50	30.21
Calcium pantothenate	>50	43.53
Nystatin	>50	47.58
Estriol	>50	55.16
Gelatine, white	>50	55.44
Triamcinolone	>50	59.83
alpha-tocopheryl acetate dry concentrate	>50	72.47
Estradiol hemihydrate	>50	74.06
Riboflavin	>50	81.64
Hyoscine hydrobromide	>50	104.50
Calcium glycerophosphate	>50	120.60
Tosylchloramide sodium	>50	128.79
Selenium yeast	>50	140.93
Carmellose sodium	>50	158.58
SyrSpend® SF Alka	>50	161.50
SyrSpend® SF pH4 neo (Maize starch)	>50	176.13
Oxalic acid	>50	189.49
Rice starch	>50	194.41
SyrSpend® SF pH4	>50	244.54
Corn starch	>50	272.47
Acacia, dried dispersion	>50	286.28
Wheat starch	>50	361.94
Potato starch	>50	368.81
Maltodextrin	>50	389.50
Fructose	>50	415.02

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cyanocobalamin / Methylcobalamin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cyanocobalamin / Methylcobalamin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cyanocobalamin	13342803	21299	40	AR-15-FG-005429-01
Caelo	Cyanocobalamin	13342807	21479	60	AR-15-FG-014917-01
Caelo	Cyanocobalamin	13342807	21479SI	30	AR-15-FG-014917-01
Caelo	Cyanocobalamin	160154	22441	60	20160309*
Caelo	Cyanocobalamin	160154	22441SI	60	20160309*
Euro OTC	Cyanocobalamin	1305040-01	21635	60	AR-15-FG-005214-01
Euro OTC	Cyanocobalamin	1506035	21867	60	20150708*
Euro OTC	Cyanocobalamin	1506035	21867SI	60	20150708*
Euro OTC	Cyanocobalamin	1506035	21872	60	0000010479
Euro OTC	Cyanocobalamin	1506035	21872SI	45	0000010479
Euro OTC	Cyanocobalamin	1604017	22536	30	20160509*
Euro OTC	Cyanocobalamin	1604017	22536SI	30	20160509*
Euro OTC	Cyanocobalamin	1812011	24465	40	20190205*
Euro OTC	Methylcobalamin	1207019-01	20743	40	1402501
Euro OTC	Methylcobalamin	1401032-01	21721	60	8778
Euro OTC	Methylcobalamin	1510002	22234	60	20151201*
Euro OTC	Methylcobalamin	1401032	22239	60	20151201*
Euro OTC	Methylcobalamin	1601043	22379	60	20160209*
Euro OTC	Methylcobalamin	1804006	24072	40	20180420*
Euro OTC	Methylcobalamin	1809001	24311	40	20180925*
Euro OTC	Methylcobalamin	1904002	24775	40	20190806*
Euro OTC	Methylcobalamin	2002014	25135	40	20200401*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1075 spectra of 22 reference samples from the substance/substance group *Cyanocobalamin / Methylcobalamin*. These samples are listed above in the *calibration samples* section. The reference samples come from 16 different batches.

- 151 887 spectra from a total of 2826 batches from further 482 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 680 spectra of 18 reference samples from the substance/substance group *Cyanocobalamin / Methylcobalamin*.
- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Cyanocobalamin	16015411	23761	40
Caelo	Cyanocobalamin	162215	23790	40
Caelo	Cyanocobalamin	21001468003	25976	40
Euro OTC	Cyanocobalamin	1907030	24965	40
Euro OTC	Cyanocobalamin	2109009	25868	50
Euro OTC	Cyanocobalamin	2206015	26272	40
Fagron	Cyanocobalamin	23H14-B07-230965	27022	40
Euro OTC	Methylcobalamin	1711031	23885	40
Euro OTC	Methylcobalamin	2006003	25412	40
Euro OTC	Methylcobalamin	2202009	26097	40
Caelo	Cyanocobalamin	13342807	21479SI†	30
Caelo	Cyanocobalamin	21001468003	25976SI	40
Euro OTC	Cyanocobalamin	1604017	22536SI†	10
Euro OTC	Cyanocobalamin	1907030	24965SI	40
Euro OTC	Cyanocobalamin	2109009	25868SI	50
Euro OTC	Cyanocobalamin	2206015	26272SI	40
Fagron	Cyanocobalamin	23H14-B07-230965	27022SI	40
Euro OTC	Methylcobalamin	2202009	26097SI	20

- 201 404 spectra from a total of 4033 batches from further 837 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 39 spectra from 25 *Apo-Ident* customers from 33 batches from the substance/substance group *Cyanocobalamin / Methylcobalamin*.
- Among them are spectra of independent samples from 33 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cyanocobalamin	19I20-B04-1955509	1
	Cyanocobalamin	20D06-B02-2016102	1
Caelo	Cyanocobalamin	16015405	1
Caelo	Cyanocobalamin	1604017-01	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cyanocobalamin	18016001	1
Caelo	Cyanocobalamin	18016010	1
Caelo	Cyanocobalamin	19088601	1
Caelo	Cyanocobalamin	19I20-B04	1
Caelo	Cyanocobalamin	21001468003	1
Caelo	Cyanocobalamin	21001468005	1
Caelo	Cyanocobalamin	9324102	1
Caelo	Cyanocobalamin	9324113	1
Caelo	Cyanocobalamin	9351704	1
Caelo	Cyanocobalamin	9373503	2
Caesar & Loretz GmbH...	Cyanocobalamin	9324102	1
Caesar & Loretz GmbH	Cyanocobalamin	16221501	1
EuRho	Cyanocobalamin	1812011-01	1
Euro OTC	Methylcobalamin	1601043-02	1
Euro OTC	Methylcobalamin	1711031-01	1
Euro OTC	Methylcobalamin	1804006-01	1
Euro OTC	Methylcobalamin	1809001-01	1
Euro OTC	Methylcobalamin	2002014-01	1
Euro OTC	Methylcobalamin	2006003-01	3
Euro OTC	Methylcobalamin	2006003-02	1
Euro OTC	Cyanocobalamin	5061204	1
Fagron	Cyanocobalamin	10K02-N05	2
Fagron	Cyanocobalamin	10K02-NO5	1
Fagron	Cyanocobalamin	13124-B01-292062	1
Fagron	Cyanocobalamin	15H31-B02-315113	1
Fagron	Cyanocobalamin	17A27-B04	1
Fagron	Cyanocobalamin	17A27-B04-339672	2
Fagron	Cyanocobalamin	B04-3396702	1
faron	Cyanocobalamin	18/10-B01-357181	1
Spinnrad/Phoenix	Cyanocobalamin	1217331032	1

- 236 028 spectra from 1515 *Apo-Ident* customers from a total of 49 225 batches from a further 720 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cyanocobalamin / Methylcobalamin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cyanocobalamin / Methylcobalamin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	1075	0	151 887
Type B	0	680	0	201 404
Type C	0	38	1	236 028

The substance/substance group *Cyanocobalamin / Methylcobalamin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.4419 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.1176 %)
Type C	100.0000 % (> 99.9007 %)	97.4359 % (> 89.7436 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20743	20743	0.00	71.31
21299	21299	0.00	52.30
21479	21479	0.00	57.69
21635	21635	0.00	45.10
21721	21721	0.00	107.55
21867	21867	0.00	46.96
21872	21872	0.00	61.16
22234	22234	0.00	40.78
22239	22239	0.00	67.66
22379	22379	0.00	55.94
22441	22441	0.00	96.37
22536	22536	0.00	88.83
24072	24072	0.00	52.17
24311	24311	0.00	60.77
24465	24465	0.00	74.85
24775	24775	0.00	73.32
25135	25135	0.00	101.46

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cyproheptadine hydrochloride 1.5 hydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	24437-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cyproheptadine hydrochloride 1.5 hydrate; Cyproheptadini hydrochloridum-1,5-hydricum

Special notes

When selecting the *Cyproheptadine hydrochloride 1.5 hydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cyproheptadine hydrochloride 1.5 hydrate	3	1	0

Second-stage model

For differentiation of the substance/substance group *Cyproheptadine hydrochloride 1.5 hydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cyproheptadine hydrochloride 1.5 hydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	134.33	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cyproheptadine hydrochloride 1.5 hydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cyproheptadine hydrochloride 1.5 hydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Cyproheptadine hydrochlor…	16K07-B01-350645	24437	40	1906179
Fagron	Cyproheptadine hydrochlor…	21H10-B06-219299	26634	40	20211207
Fagron	Cyproheptadine hydrochlor…	23G20-B01-231484	27027	40	20231025
Fagron	Cyproheptadine hydrochlor…	23G20-B01-231484	27027SI	20	20231025

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 140 spectra of 4 reference samples from the substance/substance group *Cyproheptadine hydrochloride 1.5 hydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 152 822 spectra from a total of 2839 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 3 reference samples from the substance/substance group *Cyproheptadine hydrochloride 1.5 hydrate*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Cyproheptadine hydrochlor…	20K20-B05-202444	26076	40
Fagron	Cyproheptadine hydrochlor…	20K20-B05-202444	26076SI	20
Fagron	Cyproheptadine hydrochlor…	21H10-B06-219299	26634SI†	20

- 202 004 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Cyproheptadine hydrochloride 1.5 hydrate*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cyproheptadine hydrochloride 1.5 hydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Cyproheptadine hydrochloride 1.5 hydrate and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	140	0	152 822
Type B	0	80	0	202 004
Type C	0	0	0	236 067

The substance/substance group *Cyproheptadine hydrochloride 1.5 hydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24437	24437	0.00	194.07
26634	24437	23.48	194.72
27027	24437	25.81	194.35

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cyproterone acetate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20593-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cyproterone acetate; Cyproteroni acetas

Special notes

When selecting the *Cyproterone acetate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cyproterone acetate	8	9	69

Second-stage model

For differentiation of the substance/substance group *Cyproterone acetate* the following second-stage model is used:

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cyproterone acetate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prilocaine hydrochloride	66.32	–
⋮	⋮	⋮
Oxybutynin hydrochloride	>50	84.24
Prednicarbate	>50	100.38
Amitriptyline hydrochloride	>50	123.37
Capsaicin	>50	157.62
Levocarnitine	>50	160.01
Sodium citrate	>50	205.52
Tetracaine	>50	206.95
Valine	>50	244.19
Methoxsalen	>50	343.09
Norethisterone acetate	>50	372.78
Quinine hydrochloride dihydrate	>50	385.73
Alfatradiol	>50	385.94
Pyridoxal-5-phosphate	>50	467.07
Ciprofloxacin hydrochloride	>50	511.01
Heparin sodium	>50	627.00
Triclosan	>50	1531.72
Amifampridine	>50	2159.85
Sucrose	>50	2311.03

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cyproterone acetate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cyproterone acetate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Cyproterone acetate	APCPA140201CP	23988	40	20140617
Audor Pharma	Cyproterone acetate	APX03-181002-m0C	24814	40	20181213

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cyproterone acetate	1611003	22875	40	20161201*
Euro OTC	Cyproterone acetate	1810017	24317	40	20181108*
Fagron	Cyproterone acetate	13C11-N02	21262	40	1501534
Fagron	Cyproterone acetate	13J16-No4	21985	75	1602654
Fagron	Cyproterone acetate	15I11-B01-322117	22665	40	20150921
Fagron	Cyproterone acetate	17D11-B07-333693	23238	40	20170501
Fagron	Cyproterone acetate	17D11-B07-333693	23238SI	20	20170501

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 375 spectra of 9 reference samples from the substance/substance group *Cyproterone acetate*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.
- 152 587 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 771 spectra of 24 reference samples from the substance/substance group *Cyproterone acetate*.
- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Cyproterone acetate	1903011	24609	40
Euro OTC	Cyproterone acetate	1910022	24957	40
Euro OTC	Cyproterone acetate	2003045	25270	40
Euro OTC	Cyproterone acetate	2101023	25532	40
Euro OTC	Cyproterone acetate	2205022	26192	40
Euro OTC	Cyproterone acetate	2409015	27405	40
Fagron	Cyproterone acetate	18G25-B02-352728	24289	40
Fagron	Cyproterone acetate	22I13-B01-228645	26826	40
Fagron	Cyproterone acetate	24A08-B08-235276	27178	40

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Audor Pharma	Cyproterone acetate	APCPA140201CP	23988SI†	20
Audor Pharma	Cyproterone acetate	APX03-181002-m0C	24814SI†	40
Euro OTC	Cyproterone acetate	1611003	22875SI†	30
Euro OTC	Cyproterone acetate	1810017	24317SI†	20
Euro OTC	Cyproterone acetate	1903011	24609SI	20
Euro OTC	Cyproterone acetate	1910022	24957SI	22
Euro OTC	Cyproterone acetate	2003045	25270SI	30
Euro OTC	Cyproterone acetate	2101023	25532SI	31
Euro OTC	Cyproterone acetate	2205022	26192SI	32
Euro OTC	Cyproterone acetate	2409015	27405SI	30
Fagron	Cyproterone acetate	13J16-No4	21985SI†	23
Fagron	Cyproterone acetate	15I11-B01-322117	22665SI†	33
Fagron	Cyproterone acetate	18G25-B02-352728	24289SI	20
Fagron	Cyproterone acetate	22I13-B01-228645	26826SI	30
Fagron	Cyproterone acetate	24A08-B08-235276	27178SI	30

- 201 313 spectra from a total of 4030 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 114 spectra from 65 *Apo-Ident* customers from 72 batches from the substance/substance group *Cyproterone acetate*.
- Among them are spectra of independent samples from 69 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Audor Pharma	Cyproterone acetate	APCPA140201CP	2
Audor Pharma	Cyproterone acetate	APX03-181002-m0C	1
Audor Pharma	Cyproterone acetate	cpa140201cp	1
Audor Pharma	Cyproterone acetate	X03-181002-m0C	1
Caelo	Cyproterone acetate	13j16-n04	1
Caelo	Cyproterone acetate	17D11-B07-334581	3
Caelo	Cyproterone acetate	18G25-B02-352728	1
Caelo	Cyproterone acetate	CPA150301	1
Ebert-Jacobi	Cyproterone acetate	16K09-B04-329036	1
Eu Rho/XX	Cyproterone acetate	2003045-01	2
Euro OTC	Cyproterone acetate	1502038-01	1
Euro OTC	Cyproterone acetate	2003045-01	3
Euro OTC	Cyproterone acetate	2101023-01	2
Fagron	Cyproterone acetate	11L22-N02	1
Fagron	Cyproterone acetate	12D02-N13	1
Fagron	Cyproterone acetate	12F25-N09	3
Fagron	Cyproterone acetate	12J24-N02	1
Fagron	Cyproterone acetate	12L19-N05	3
Fagron	Cyproterone acetate	13/09-N03	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Cyproterone acetate	13/16-N04	2
Fagron	Cyproterone acetate	13j16n04	1
Fagron	Cyproterone acetate	13J16-N04	2
Fagron	Cyproterone acetate	13j16-no4	1
Fagron	Cyproterone acetate	15H04-B06-311064	1
Fagron	Cyproterone acetate	15I11-B01-315381	2
Fagron	Cyproterone acetate	16K09-B04-329037	1
Fagron	Cyproterone acetate	17D11-B07	1
Fagron	Cyproterone acetate	17D11-B07-336729	2
Fagron	Cyproterone acetate	17D11-B07-338440	1
Fagron	Cyproterone acetate	18041805	1
Fagron	Cyproterone acetate	18B05_B05_346309	1
Fagron	Cyproterone acetate	18B05-346308	1
Fagron	Cyproterone acetate	18B05-B05-346307	1
Fagron	Cyproterone acetate	18B05-B05-346309	3
Fagron	Cyproterone acetate	18G25-B02	1
Fagron	Cyproterone acetate	18G25-B02-352307	2
Fagron	Cyproterone acetate	18G25-B02-352728	3
Fagron	Cyproterone acetate	18G25-B02-354474	1
Fagron	Cyproterone acetate	18G25-B02-354475	3
Fagron	Cyproterone acetate	18G25-B02-354476	1
Fagron	Cyproterone acetate	18G25-B02-355388	2
Fagron	Cyproterone acetate	18G25-B02-358855	3
Fagron	Cyproterone acetate	18G25-B02-358856	4
Fagron	Cyproterone acetate	18G25-B02-358857	1
Fagron	Cyproterone acetate	19A23-B04	2
Fagron	Cyproterone acetate	19A23-B04_363300	1
Fagron	Cyproterone acetate	19A23-B04-363299	1
Fagron	Cyproterone acetate	19a23-b04-363300	1
Fagron	Cyproterone acetate	19A23-B04-363300	2
Fagron	Cyproterone acetate	19A23-B04-363301	1
Fagron	Cyproterone acetate	19A23-B04-363302	1
Fagron	Cyproterone acetate	19A23B04367910	1
Fagron	Cyproterone acetate	19A23-B04367910	1
Fagron	Cyproterone acetate	19A23-B04-367910	3
Fagron	Cyproterone acetate	19A23-B04-363301	1
Fagron	Cyproterone acetate	19A23-B04-367910	1
Fagron	Cyproterone acetate	20101807	1
Fagron	Cyproterone acetate	20K11-F01	1
Fagron	Cyproterone acetate	20K11-F01-376805	1
Fagron	Cyproterone acetate	20K11-F01-376807	1
Fagron	Cyproterone acetate	21F22-B04-213628	4
Fagron	Cyproterone acetate	21J12-B02-215671	1
Fagron	Cyproterone acetate	21L17-B02	2
Fagron	Cyproterone acetate	21L17-B02-217596	1
Fagron	Cyproterone acetate	21L17-B02-217628	1
Fagron	Cyproterone acetate	22113-B01-228645	1
Fagron	Cyproterone acetate	2OK11-F01-376805	1
Fagron	Cyproterone acetate	2OK11-FO1-376805	1
Fagron	Cyproterone acetate	8B11-N06	1
Fagron	Cyproterone acetate	B0392/110020	3
Fagron	Cyproterone acetate	B04-3664709	1
Fagron	Cyproterone acetate	EU-CPA-170301	1
Fargon/Noweda	Cyproterone acetate	18G25-B02-352729	1
Fargon/Noweda	Cyproterone acetate	18G25-B02-354476	1
Gehe	Cyproterone acetate	22I13-B01-228645	1
Sanacorp	Cyproterone acetate	18B05-B05-346307	1

- 235 953 spectra from 1515 *Apo-Ident* customers from a total of 49 186 batches from a further

721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cyproterone acetate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cyproterone acetate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	375	0	152 587
Type B	0	771	0	201 313
Type C	0	114	0	235 953

The substance/substance group *Cyproterone acetate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2218 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 94.7368 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21262	21262	0.00	109.91
21985	21985	0.00	110.79
22665	21985	2.72	115.03
22875	22875	0.00	112.37
23238	21985	3.72	109.72
23988	21985	2.56	109.74
24317	24317	0.00	110.75
24814	21985	3.97	112.70

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cysteine hydrochloride monohydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20530-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cysteine hydrochloride monohydrate; Cysteini hydrochloridum monohydricum

Special notes

When selecting the *Cysteine hydrochloride monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cysteine hydrochloride monohydrate	9	4	4

Second-stage model

For differentiation of the substance/substance group *Cysteine hydrochloride monohydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cysteine hydrochloride monohydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	102.76	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cysteine hydrochloride monohydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cysteine hydrochloride monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cysteine hydrochloride mo…	1701012	23003	40	20170207*
Euro OTC	Cysteine hydrochloride mo…	1706023	23548	40	20170721*
Euro OTC	Cysteine hydrochloride mo…	1807010-01	24188	40	20180808
Euro OTC	Cysteine hydrochloride mo…	1901012	24482	40	20190206*
Euro OTC	Cysteine hydrochloride mo…	2010020	25453	40	20201216*
Euro OTC	Cysteine hydrochloride mo…	2205018	26186	40	20220613*
Euro OTC	Cysteine hydrochloride mo…	2205018	26186SI	20	20220613*
Euro OTC	Cysteine hydrochloride mo…	2301029	26863	40	20230728*
Euro OTC	Cysteine hydrochloride mo…	2301029	26863SI	20	20230728*
Euro OTC	Cysteine hydrochloride mo…	2407009	27402	40	20241105*
Euro OTC	Cysteine hydrochloride mo…	2407009	27402SI	20	20241105*
Fagron	Cysteine hydrochloride mo…	22J13-B02	26447	40	20221207*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 420 spectra of 12 reference samples from the substance/substance group *Cysteine hydrochloride monohydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 542 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 4 reference samples from the substance/substance group *Cysteine hydrochloride monohydrate*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Cysteine hydrochloride mo…	1304019-01	21325	40
Euro OTC	Cysteine hydrochloride mo…	1507006	21840	60
Euro OTC	Cysteine hydrochloride mo…	1510015	21941	60
Euro OTC	Cysteine hydrochloride mo…	1603018	22516	40

- 201 884 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 8 spectra from 4 *Apo-Ident* customers from 5 batches from the substance/substance group *Cysteine hydrochloride monohydrate*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Cysteine hydrochloride mo…	1304019-01	1
Euro OTC	Cysteine hydrochloride mo…	1807010-01	3
Euro OTC	Cysteine hydrochloride mo…	180710-01	1
Euro OTC	Cysteine hydrochloride mo…	1901012-01	1
Euro OTC	Cysteine hydrochloride mo…	2010020-01	2

- 236 059 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cysteine hydrochloride monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cysteine hydrochloride monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	200	0	201 884
Type C	0	8	0	236 059

The substance/substance group *Cysteine hydrochloride monohydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23003	23003	0.00	198.00
23548	23548	0.00	199.65

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24188	24482	7.82	197.97
24482	24482	0.00	201.91
25453	25453	0.00	196.71
26186	26186	0.00	198.65
26447	26447	0.00	205.64
26863	26863	0.00	202.24
27402	27402	0.00	205.98

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Cystine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20515-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Cystine; Cystinum

Special notes

When selecting the *Cystine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Cystine	8	5	15

Second-stage model

For differentiation of the substance/substance group *Cystine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Cystine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Lysine hydrochloride	83.37	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Cystine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Cystine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Cystine	1307052-01	21328	40	20130918
Euro OTC	Cystine	1408016-01	21715	60	20140911
Euro OTC	Cystine	1603010	22523	40	20160406*
Euro OTC	Cystine	1610013	22863	40	20161110*
Euro OTC	Cystine	1801016	23879	40	20180126*
Euro OTC	Cystine	2009038	25411	40	20201020*
Euro OTC	Cystine	2305001	26876	40	20230802*
Fagron	Cystine	15F08-B05-310685	23767	40	20150616

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 340 spectra of 8 reference samples from the substance/substance group *Cystine*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 622 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 230 spectra of 7 reference samples from the substance/substance group *Cystine*.
- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Cystine	1811005	24332	40
Euro OTC	Cystine	1904022	24617	40
Euro OTC	Cystine	1910028	24933	40
Euro OTC	Cystine	2202004	26036	40
Euro OTC	Cystine	2207020	26435	40
Euro OTC	Cystine	2202004	26036SI	10
Euro OTC	Cystine	2305001	26876SI†	20

- 201 854 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 32 spectra from 9 *Apo-Ident* customers from 16 batches from the substance/substance group *Cystine*.
- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Cystine	190402201	1
Euro OTC	Cystine	1204090	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cystine	1207013-01	2
Euro OTC	Cystine	1801016-01	3
Euro OTC	Cystine	1811005-01	2
Euro OTC	Cystine	1904022-01	1
Euro OTC	Cystine	1910028-01	1
Euro OTC	Cystine	2009038-01	4
Euro OTC	Cystine	2009038-02	3
Euro OTC	Cystine	2081301	1
Euro OTC	Cystine	2202004-01	3
Euro OTC	Cystine	26081408	1
Euro OTC	Cystine	30041809	1
Euro OTC	Cystine	3021502	1
Fagron	Cystine	12D26-B04-285823	2
Fagron	Cystine	15F08-B05-310685	1
Fagron	Cystine	1904022-01	1
Fagron	Cystine	1910028-01	3

- 236 035 spectra from 1515 *Apo-Ident* customers from a total of 49 242 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Cystine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Cystine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	340	0	152 622
Type B	0	230	0	201 854
Type C	0	32	0	236 035

The substance/substance group *Cystine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2353 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.3913 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 81.2500 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21328	23879	5.84	137.53
21715	22523	5.26	136.70
22523	22523	0.00	138.53
22863	22863	0.00	141.69
23767	23879	12.20	141.71
23879	23879	0.00	140.07
25411	25411	0.00	136.69
26876	26876	0.00	152.48

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Dequalinium chloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20350-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dequalinium chloride; Dequalinii chloridum

Special notes

When selecting the *Dequalinium chloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Dequalinium chloride	13	7	129

Second-stage model

For differentiation of the substance/substance group *Dequalinium chloride* the following second-stage model is used:

- Submodel 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Dequalinium chloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	72.04	–
⋮	⋮	⋮
Dithranol	>50	59.83
Eosin Y	>50	96.32
Oxytetracycline hydrochloride	>50	133.02
Sodium salicylate	>50	143.24
Levothyroxin sodium	>50	184.62
Tannin	>50	252.26
Acetylsalicylic acid	>50	255.42
Benzoic acid	>50	433.75

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Dequalinium chloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Dequalinium chloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dequalinium chloride	12361908	21296	40	1412076
Caelo	Dequalinium chloride	12361906	21387	60	20121228
Caelo	Dequalinium chloride	15218406	22953	40	20150622
Caelo	Dequalinium chloride	15402803	23121	40	1707614
Caelo	Dequalinium chloride	154028	23362	40	20160219*
Caelo	Dequalinium chloride	154028	24403	40	20160219*
Caelo	Dequalinium chloride	191314	25205	40	20190626*
Euro OTC	Dequalinium chloride	1405012-01	21617	60	20140623
Euro OTC	Dequalinium chloride	1512032	22295	60	20160121*
Euro OTC	Dequalinium chloride	1512032-02	24142	40	1809202
Euro OTC	Dequalinium chloride	2003008	25156	40	20200528*
Euro OTC	Dequalinium chloride	2103018	25687	40	20210421*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Dequalinium chloride	13I26-N10	21269	40	20130121
Fagron	Dequalinium chloride	15B16-B04-332113	23266	40	20150226

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 620 spectra of 14 reference samples from the substance/substance group *Dequalinium chloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 13 different batches.

- 152 342 spectra from a total of 2829 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 500 spectra of 12 reference samples from the substance/substance group *Dequalinium chloride*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Dequalinium chloride	180794	24011	40
Caelo	Dequalinium chloride	22001564	26243	40
Caelo	Dequalinium chloride	24001318	27314	40
Euro OTC	Dequalinium chloride	1804009	24082	40
Euro OTC	Dequalinium chloride	2310016	27194	40
Fagron	Dequalinium chloride	11D29-N11	20660	80
Fagron	Dequalinium chloride	19J16-B08-197304	25177	40
Caelo	Dequalinium chloride	12361906	21386	60
Caelo	Dequalinium chloride	12361906	21387†	60
Caelo	Dequalinium chloride	22001564	26243SI	20
Caelo	Dequalinium chloride	24001318	27314SI	20
Euro OTC	Dequalinium chloride	2310016	27194SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 584 spectra from a total of 4037 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 498 spectra from 309 *Apo-Ident* customers from 138 batches from the substance/substance group *Dequalinium chloride*.
- Among them are spectra of independent samples from 124 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Dequalinium chloride	20003344009	1
	Dequalinium chloride	20003344010	2
	Dequalinium chloride	2103018-01	3
	Dequalinium chloride	22001564003	2
	Dequalinium chloride	22001564004	2
	Dequalinium chloride	22001564008	1
	Dequalinium chloride	22001564013	1
AHD	Dequalinium chloride	15218401	1
Alliance H.	Dequalinium chloride	1512032-01	1
Alliance Health	Dequalinium chloride	12077508	1
Alliance Healthcare	Dequalinium chloride	19131402	1
Alliance Healthcare	Dequalinium chloride	2003008-01	1
Allianz Healthcare	Dequalinium chloride	1512032-01	1
Anzag ek:7.89EUR	Dequalinium chloride	11166204	1
Anzag	Dequalinium chloride	15B16-B04-340177	1
apomix	Dequalinium chloride	1804009-01	1
Caelo	Dequalinium chloride		1
Caelo	Dequalinium chloride	10879409	1
Caelo	Dequalinium chloride	11166203	1
Caelo	Dequalinium chloride	11166204	2
Caelo	Dequalinium chloride	11166209	1
Caelo	Dequalinium chloride	12077508	2
Caelo	Dequalinium chloride	12077510	7
Caelo	Dequalinium chloride	1210008-03	1
Caelo	Dequalinium chloride	12361906	3
Caelo	Dequalinium chloride	12361908	2
Caelo	Dequalinium chloride	12361911	3
Caelo	Dequalinium chloride	12G05-N07	1
Caelo	Dequalinium chloride	13/26-N10	1
Caelo	Dequalinium chloride	13348805	2
Caelo	Dequalinium chloride	13A23-N02	2
Caelo	Dequalinium chloride	1405012-02	1
Caelo	Dequalinium chloride	14072901	1
Caelo	Dequalinium chloride	14C10-B03	1
Caelo	Dequalinium chloride	151203202	1
Caelo	Dequalinium chloride	1512032-02	3
Caelo	Dequalinium chloride	152184	1
Caelo	Dequalinium chloride	15218401	7

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dequalinium chloride	15218402	1
Caelo	Dequalinium chloride	15218404	2
Caelo	Dequalinium chloride	15218406	6
Caelo	Dequalinium chloride	15218407	1
Caelo	Dequalinium chloride	15218410	1
Caelo	Dequalinium chloride	15402801	3
Caelo	Dequalinium chloride	15402803	4
Caelo	Dequalinium chloride	15402805	2
Caelo	Dequalinium chloride	15402806	2
Caelo	Dequalinium chloride	15402807	2
Caelo	Dequalinium chloride	15B16-B04	1
Caelo	Dequalinium chloride	15B16-B04-326872	1
Caelo	Dequalinium chloride	15B16-B04-337594	1
Caelo	Dequalinium chloride	15B16-B04-342302	1
Caelo	Dequalinium chloride	18015801	2
Caelo	Dequalinium chloride	18015802	2
Caelo	Dequalinium chloride	1804009-03	2
Caelo	Dequalinium chloride	18079402	1
Caelo	Dequalinium chloride	18079403	6
Caelo	Dequalinium chloride	18079404	3
Caelo	Dequalinium chloride	18079405	1
Caelo	Dequalinium chloride	18079407	3
Caelo	Dequalinium chloride	18079408	1
Caelo	Dequalinium chloride	18079410	1
Caelo	Dequalinium chloride	18079411	3
Caelo	Dequalinium chloride	191314003	8
Caelo	Dequalinium chloride	191314004	6
Caelo	Dequalinium chloride	191314005	1
Caelo	Dequalinium chloride	191314006	2
Caelo	Dequalinium chloride	19131402	10
Caelo	Dequalinium chloride	20003344004	6
Caelo	Dequalinium chloride	20003344006	1
Caelo	Dequalinium chloride	20003344007	2
Caelo	Dequalinium chloride	20003344009	2
Caelo	Dequalinium chloride	20003344012	3
Caelo	Dequalinium chloride	2000334404	1
Caelo	Dequalinium chloride	2003008-01	2
Caelo	Dequalinium chloride	215I-01325	1
Caelo	Dequalinium chloride	22001564002	1
Caelo	Dequalinium chloride	220812K2	1
Caelo	Dequalinium chloride	3613A-01325	1
Caelo	Dequalinium chloride	5315I-01325	1
Caeol/Noweda	Dequalinium chloride	19131402	2
Caesar & Loretz GmbH...	Dequalinium chloride	18079411	1
Caesar & Loretz GmbH...	Dequalinium chloride	191314007	1
Caesar & Loretz GmbH...	Dequalinium chloride	20003344003	1
Caesar & Loretz GmbH...	Dequalinium chloride	20003344007	1
Caesar & Loretz GmbH	Dequalinium chloride	18079404	2
Caesar & Loretz GmbH	Dequalinium chloride	18079410	1
Caesar & Loretz GmbH	Dequalinium chloride	18079411	1
Caesar & Loretz GmbH	Dequalinium chloride	191314003	3
Caesar & Loretz GmbH	Dequalinium chloride	191314004	1
Caesar & Loretz GmbH	Dequalinium chloride	191314006	2
Caesar & Loretz GmbH	Dequalinium chloride	191314007	3
Caesar & Loretz GmbH	Dequalinium chloride	19131402	5
Caesar & Loretz GmbH	Dequalinium chloride	20003344004	2
Caesar & Loretz GmbH	Dequalinium chloride	210008690091	1
Caesar & Loretz GmbH	Dequalinium chloride	22001564002	1
Cealo, GEHE	Dequalinium chloride	2003008-01	1
Eurho Sanacorp	Dequalinium chloride	2003008-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho/ Anzag	Dequalinium chloride	220627(2103018-01)	1
EuRho/ Anzag	Dequalinium chloride	80(1804009-01)	1
EuRho/Gehe	Dequalinium chloride	2003008-01	2
EuRho/Phoenix	Dequalinium chloride	2103018-01	1
EuRho	Dequalinium chloride	1110002-01	1
EuRho	Dequalinium chloride	2003008-01	1
Euro OTC	Dequalinium chloride		3
Euro OTC	Dequalinium chloride	1010022-01	2
Euro OTC	Dequalinium chloride	1103045-01	1
Euro OTC	Dequalinium chloride	11091701	1
Euro OTC	Dequalinium chloride	1110002-01	2
Euro OTC	Dequalinium chloride	1210008-01	2
Euro OTC	Dequalinium chloride	1210008-02	2
Euro OTC	Dequalinium chloride	1210008-03	2
Euro OTC	Dequalinium chloride	1405012-01	5
Euro OTC	Dequalinium chloride	1405012-02	6
Euro OTC	Dequalinium chloride	1407029-01	7
Euro OTC	Dequalinium chloride	1407029-02	6
Euro OTC	Dequalinium chloride	15061204	1
Euro OTC	Dequalinium chloride	151203201	1
Euro OTC	Dequalinium chloride	1512032-01	21
Euro OTC	Dequalinium chloride	1512032-02	13
Euro OTC	Dequalinium chloride	180400901	1
Euro OTC	Dequalinium chloride	1804009-01	20
Euro OTC	Dequalinium chloride	1804009-02	4
Euro OTC	Dequalinium chloride	1804009-03	22
Euro OTC	Dequalinium chloride	18040092-02	1
Euro OTC	Dequalinium chloride	18044009-01	1
Euro OTC	Dequalinium chloride	2000300801	1
Euro OTC	Dequalinium chloride	20030008-01	1
Euro OTC	Dequalinium chloride	2003008-01	23
Euro OTC	Dequalinium chloride	2103018-01	20
Euro OTC	Dequalinium chloride	210318-01	1
Euro OTC	Dequalinium chloride	211118(2003008)	1
Euro OTC	Dequalinium chloride	220809(2103018-01)	1
Euro OTC	Dequalinium chloride	804009-021	1
Euro OTC	Dequalinium chloride	81(1804009-01)	1
Euro OTC	Dequalinium chloride	EuroOTC	1
Euro/Sanacorp	Dequalinium chloride	1512032-02	1
Euro/Spangro	Dequalinium chloride	1512032-02	1
Fag / Noweda	Dequalinium chloride	15B16-B04-321326	1
Fagron	Dequalinium chloride		5
Fagron	Dequalinium chloride	10H05-N07	1
Fagron	Dequalinium chloride	12B14-N01	1
Fagron	Dequalinium chloride	12D05-N09	1
Fagron	Dequalinium chloride	12G05-N07	2
Fagron	Dequalinium chloride	13A23-N02	3
Fagron	Dequalinium chloride	13D26-N06	3
Fagron	Dequalinium chloride	13I26-N10	1
Fagron	Dequalinium chloride	1407029-01	2
Fagron	Dequalinium chloride	14C10-B03	1
Fagron	Dequalinium chloride	14C10B03292286	1
Fagron	Dequalinium chloride	14C10-B03-292286	4
Fagron	Dequalinium chloride	15B16-B04	2
Fagron	Dequalinium chloride	15B16B04304432	1
Fagron	Dequalinium chloride	15B16-B04-304432	2
Fagron	Dequalinium chloride	15B16-B04-316267	4
Fagron	Dequalinium chloride	15B16B04321326	1
Fagron	Dequalinium chloride	15B16-B04-321326	1
Fagron	Dequalinium chloride	15B16-B04-326872	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Dequalinium chloride	15B16-B04-332113	3
Fagron	Dequalinium chloride	15B16B04337594	1
Fagron	Dequalinium chloride	15B16-B04-340177	1
Fagron	Dequalinium chloride	15B16-B04-342302	2
Fagron	Dequalinium chloride	15B16-B04-346969	4
Fagron	Dequalinium chloride	15B16-B04-352989	2
Fagron	Dequalinium chloride	15B16-B04-354618	2
Fagron	Dequalinium chloride	18B16-B04-356149	1
Fagron	Dequalinium chloride	19J16-B08	4
Fagron	Dequalinium chloride	19J16B08197304	2
Fagron	Dequalinium chloride	19J16-B08-197304	8
Fagron	Dequalinium chloride	19JI-B08-197304	1
Fagron	Dequalinium chloride	20F19-B03-201436	6
Fagron	Dequalinium chloride	20I18-B01-202442	2
Fagron	Dequalinium chloride	B03_2014306	1
Fagron	Dequalinium chloride	B03-2014306	3
Fiebig	Dequalinium chloride	2003008-01	1
Gatt-Koller	Dequalinium chloride	1800212	1
GEHE/ EuRho	Dequalinium chloride	2103018-01	1
Gehe/EuRho	Dequalinium chloride	9245-90125	1
Gehe	Dequalinium chloride	1512032-01	1
GEHE	Dequalinium chloride	1804009-01	1
GUMO	Dequalinium chloride	191314003	1
Klosterring	Dequalinium chloride	15B16-B04-321326	1
L30	Dequalinium chloride	1804009-01	1
Lamotte/Spangroh	Dequalinium chloride	15218404	1
Lebsa/AHD	Dequalinium chloride	1405012-01	1
LEBSA/Phoenix	Dequalinium chloride	1210008-03	1
LEBSA	Dequalinium chloride		1
Lebsa	Dequalinium chloride	2003008-01	2
Nachprüfung	Dequalinium chloride	2082019-10	1
Noweda	Dequalinium chloride	12b14-n05	1
Ph.Euro/Noweda	Dequalinium chloride	2103018-01	1
Phoenix	Dequalinium chloride	191314006	1
Phönix/EuRo	Dequalinium chloride	2003008-01	1
Phönix/Fagon	Dequalinium chloride	15B16-B04-316267	1
Phönix	Dequalinium chloride	10127-N02Retest	1
Phönix	Dequalinium chloride	1110002-01	1
Phönix	Dequalinium chloride	13D26-N06	1
Phönix	Dequalinium chloride	151203201	1
Phönix	Dequalinium chloride	1804009-01	1
phönix	Dequalinium chloride	2103018-01	1
Raben-Apotheke Mildenau	Dequalinium chloride	1405012-01	1
S.Binder	Dequalinium chloride	1210008-04	1
Sanacorp	Dequalinium chloride	18079407	2
Sanacorp	Dequalinium chloride	19131402	1
Th. Geyer	Dequalinium chloride	15B16-B04-354618	1
Wepa Apothekenbedarf	Dequalinium chloride	151203202	1

- 235 569 spectra from 1515 *Apo-Ident* customers from a total of 49 121 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dequalinium chloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose,

all relevant spectra of the various substances were compared with *Dequalinium chloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	620	0	152 342
Type B	0	500	0	201 584
Type C	0	497	1	235 569

The substance/substance group *Dequalinium chloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0323 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8000 %)
Type C	100.0000 % (> 99.9007 %)	99.7992 % (> 99.1968 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21269	21296	50.39	149.16
21296	21296	0.00	170.94
21387	21296	13.94	174.93
21617	21296	28.41	190.82
22295	22295	0.00	203.31
22953	21296	38.21	152.53
23121	23121	0.00	268.13
23266	23362	38.27	233.54
23362	23362	0.00	213.82
24142	24142	0.00	144.92
24403	24403	0.00	163.84
25156	25156	0.00	258.31
25205	25205	0.00	152.61
25687	25687	0.00	246.45

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Dexamethasone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20009-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dexamethasone; Dexamethasonum

Special notes

When selecting the *Dexamethasone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Dexamethasone	10	17	387

Second-stage model

For differentiation of the substance/substance group *Dexamethasone* the following second-stage model is used:

- Submodel 02

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Dexamethasone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prednisolon dihydrogen phosphate di…	67.36	–
⋮	⋮	⋮
Betamethasone	>50	34.36
Prednisolone	>50	39.87
Fluocinolone acetonide	>50	51.18
Triamcinolone acetonide	>50	57.26
Methylprednisolone	>50	68.95
Tyrothricin	>50	135.68
Gramicidin	>50	184.52

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Dexamethasone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Dexamethasone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dexamethasone	13084315	21403	60	AR-15-FG-006810-01
Caelo	Dexamethasone	15054627	23169	40	20150420
Caelo	Dexamethasone	190221	24504	40	20190214*
Caelo	Dexamethasone	190221	24504SI	40	20190214*
Caelo	Dexamethasone	23002226	26967	40	20230922*
Euro OTC	Dexamethasone	1303007-01	21289	40	1407432
Euro OTC	Dexamethasone	1303007-01	21850	60	20130328
Euro OTC	Dexamethasone	1601052	22364	45	20160225*
Euro OTC	Dexamethasone	1601052	22364SI	45	20160225*
Euro OTC	Dexamethasone	1611001	22914	40	20161212*
Euro OTC	Dexamethasone	1611001	22914SI	37	20161212*
Euro OTC	Dexamethasone	2005024	25301	40	20200824*
Fagron	Dexamethasone	16F02-B05-324844	23168	40	20160711
Fagron	Dexamethasone	19A24-B01-361445	24705	40	20190403

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 607 spectra of 14 reference samples from the substance/substance group *Dexamethasone*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.
- 152 355 spectra from a total of 2832 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1518 spectra of 38 reference samples from the substance/substance group *Dexamethasone*.
- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Dexamethasone	13084306	21062	60
Caelo	Dexamethasone	171042	23331	40
Caelo	Dexamethasone	172856	23841	40
Caelo	Dexamethasone	190865	24742	40
Caelo	Dexamethasone	20002251	25633	40
Caelo	Dexamethasone	21001380	25795	40
Caelo	Dexamethasone	22000049	25996	40
Caelo	Dexamethasone	22002762	26476	40
Euro OTC	Dexamethasone	1209008-02	21078	60
Euro OTC	Dexamethasone	1708004	23692	40
Euro OTC	Dexamethasone	1806023	24136	40
Euro OTC	Dexamethasone	1909011	24839	40
Euro OTC	Dexamethasone	1708004-02	24867	40
Euro OTC	Dexamethasone	2109019	25874	50
Euro OTC	Dexamethasone	2208005	26264	40
Fagron	Dexamethasone	19A24-B01-359626	24573	40
Fagron	Dexamethasone	22A17-B06-218167	26074	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Dexamethasone	15054627	23169SI†	20
Caelo	Dexamethasone	171042	23331SI	24
Caelo	Dexamethasone	172856	23841SI	40
Caelo	Dexamethasone	190865	24742SI	40
Caelo	Dexamethasone	20002251	25633SI	40
Caelo	Dexamethasone	21001380	25795SI	40
Caelo	Dexamethasone	22000049	25996SI	40
Caelo	Dexamethasone	22002762	26476SI	40
Caelo	Dexamethasone	23002226	26967SI†	40
Euro OTC	Dexamethasone	1303007-01	21850SI†	45
Euro OTC	Dexamethasone	1708004	23692SI	26
Euro OTC	Dexamethasone	1806023	24136SI	33
Euro OTC	Dexamethasone	1909011	24839SI	40
Euro OTC	Dexamethasone	1708004-02	24867SI	40
Euro OTC	Dexamethasone	2005024	25301SI†	40
Euro OTC	Dexamethasone	2109019	25874SI	50
Euro OTC	Dexamethasone	2208005	26264SI	40
Fagron	Dexamethasone	16F02-B05-324844	23168SI†	30
Fagron	Dexamethasone	19A24-B01-359626	24573SI	40
Fagron	Dexamethasone	19A24-B01-361445	24705SI†	40
Fagron	Dexamethasone	22A17-B06-218167	26074SI	40

- 200 566 spectra from a total of 4022 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2898 spectra from 954 *Apo-Ident* customers from 400 batches from the substance/substance group *Dexamethasone*.

- Among them are spectra of independent samples from 386 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Dexamethasone	2005024-03	1
	Dexamethasone	2109019	1
	Dexamethasone	2109019-01	2
	Dexamethasone	2109019-03	4
	Dexamethasone	22000049004	1
	Dexamethasone	22000049005	3
	Dexamethasone	22000049009	2
	Dexamethasone	22000049011	2
	Dexamethasone	2200043005	1
	Dexamethasone	2200276005	1
	Dexamethasone	22002762003	5
	Dexamethasone	22002762004	3
	Dexamethasone	22002762005	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Dexamethasone	22002762008	8
	Dexamethasone	22002762009	5
	Dexamethasone	22002762010	2
	Dexamethasone	22002762011	2
	Dexamethasone	22002762014	2
	Dexamethasone	22002762015	7
	Dexamethasone	22002762016	8
	Dexamethasone	22002762017	2
	Dexamethasone	2202762005	1
	Dexamethasone	2202762017	1
	Dexamethasone	2208005-01	10
	Dexamethasone	2208005-02	1
	Dexamethasone	2208005-03	1
	Dexamethasone	22B26-B06-222195	2
	Dexamethasone	23B23-B03220800	1
	Dexamethasone	23B-23-B03-220800	1
07.2021	Dexamethasone	1909011	1
AHC	Dexamethasone	22002762016	1
AHD	Dexamethasone	17104210	1
AHD	Dexamethasone	17104211	1
AHD	Dexamethasone	17L19-B03-344099	1
AHD	Dexamethasone	1806023-01	1
AHD	Dexamethasone	19022108	1
AHD	Dexamethasone	1909011-01	1
AHD	Dexamethasone	21001380002	1
AHD	Dexamethasone	22002762008	1
AHD	Dexamethasone	22002762015	1
AHD	Dexamethasone	2208005-01	1
ALH	Dexamethasone	15054617	2
Alliance Healthcare	Dexamethasone	20003905004	1
Alliance/Caeolo	Dexamethasone	19086503	1
Alliance/EuRho	Dexamethasone	1909011-02	1
Alliance	Dexamethasone	22002762005	1
alliance	Dexamethasone	22002762008	1
Alliance	Dexamethasone	22002762016	1
Anzag	Dexamethasone	1233305	1
Anzag	Dexamethasone	17332404	1
Anzag	Dexamethasone	2200004909	1
Anzag	Dexamethasone	22002762005	1
Apo ident	Dexamethasone	1909011-02	2
Apo ident	Dexamethasone	2005024-03	1
apomix	Dexamethasone	1611001-01	1
Bombastus	Dexamethasone	150546629	1
Bombastus	Dexamethasone	17332418	1
Bombastus	Dexamethasone	1806023-01	1
BUFA	Dexamethasone	97A29FP-101103	2
Cael / GEHE	Dexamethasone	19086513	1
Caelo	Dexamethasone		3
Caelo	Dexamethasone	10369920	8
Caelo	Dexamethasone	10369921	2
Caelo	Dexamethasone	11105502	1
Caelo	Dexamethasone	111055-02	1
Caelo	Dexamethasone	117019022107	1
Caelo	Dexamethasone	117117332419	1
Caelo	Dexamethasone	1203304788	1
Caelo	Dexamethasone	12033301	3
Caelo	Dexamethasone	12033303	1
Caelo	Dexamethasone	12033304	1
Caelo	Dexamethasone	12033305	4
Caelo	Dexamethasone	12033307	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dexamethasone	12033308	2
Caelo	Dexamethasone	12033312	2
Caelo	Dexamethasone	12033314	7
Caelo	Dexamethasone	12033315	4
Caelo	Dexamethasone	12033317	5
Caelo	Dexamethasone	12033318	4
Caelo	Dexamethasone	1209008-01	1
Caelo	Dexamethasone	12091306	1
Caelo	Dexamethasone	12165803	1
Caelo	Dexamethasone	12165804	1
Caelo	Dexamethasone	1303007-03	1
Caelo	Dexamethasone	13084304	2
Caelo	Dexamethasone	13084305	5
Caelo	Dexamethasone	13084306	3
Caelo	Dexamethasone	13084307	2
Caelo	Dexamethasone	13084308	2
Caelo	Dexamethasone	13084309	1
Caelo	Dexamethasone	13084310	8
Caelo	Dexamethasone	13084313	4
Caelo	Dexamethasone	13084316	4
Caelo	Dexamethasone	13084317	7
Caelo	Dexamethasone	13084319	5
Caelo	Dexamethasone	13084320	2
Caelo	Dexamethasone	130854306	1
Caelo	Dexamethasone	13342310	1
Caelo	Dexamethasone	1335213	1
Caelo	Dexamethasone	13352302	9
Caelo	Dexamethasone	13352303	1
Caelo	Dexamethasone	13352304	1
Caelo	Dexamethasone	13352308	7
Caelo	Dexamethasone	13352309	2
Caelo	Dexamethasone	13352310	17
Caelo	Dexamethasone	13352311	1
Caelo	Dexamethasone	13352312	15
Caelo	Dexamethasone	13352315	2
Caelo	Dexamethasone	13D12-N09	1
Caelo	Dexamethasone	13G08-N13	2
Caelo	Dexamethasone	14196402	3
Caelo	Dexamethasone	1504610	1
Caelo	Dexamethasone	1504618	1
Caelo	Dexamethasone	1504631	1
Caelo	Dexamethasone	15054506	1
Caelo	Dexamethasone	15054602	7
Caelo	Dexamethasone	15054603	3
Caelo	Dexamethasone	15054605	11
Caelo	Dexamethasone	15054606	14
Caelo	Dexamethasone	15054609	5
Caelo	Dexamethasone	15054610	1
Caelo	Dexamethasone	15054611	7
Caelo	Dexamethasone	15054614	5
Caelo	Dexamethasone	15054616	6
Caelo	Dexamethasone	15054617	11
Caelo	Dexamethasone	15054618	3
Caelo	Dexamethasone	15054620/170314D	1
Caelo	Dexamethasone	15054621	9
Caelo	Dexamethasone	15054622	35
Caelo	Dexamethasone	15054623	10
Caelo	Dexamethasone	15054627	2
Caelo	Dexamethasone	15054628	11
Caelo	Dexamethasone	15054629	20

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dexamethasone	15054631	6
Caelo	Dexamethasone	1505623	1
Caelo	Dexamethasone	15215601	1
Caelo	Dexamethasone	15A05-B01-304637	1
Caelo	Dexamethasone	15I04-B04-315528	1
Caelo	Dexamethasone	15K17-B07-321457	1
Caelo	Dexamethasone	1601052-01	1
Caelo	Dexamethasone	1601052-02	3
Caelo	Dexamethasone	16012207	1
Caelo	Dexamethasone	160821D	1
Caelo	Dexamethasone	161001-01	1
Caelo	Dexamethasone	1611001-01	3
Caelo	Dexamethasone	16K24-B05-330281	1
Caelo	Dexamethasone	1704203	1
Caelo	Dexamethasone	1704204	1
Caelo	Dexamethasone	1708004-01	10
Caelo	Dexamethasone	17081716	1
Caelo	Dexamethasone	1708804-01	1
Caelo	Dexamethasone	17104201	1
Caelo	Dexamethasone	17104202	2
Caelo	Dexamethasone	17104203	6
Caelo	Dexamethasone	17104204	9
Caelo	Dexamethasone	17104205	8
Caelo	Dexamethasone	17104210	24
Caelo	Dexamethasone	17104211	30
Caelo	Dexamethasone	17104212	2
Caelo	Dexamethasone	17104216	12
Caelo	Dexamethasone	171042165511	1
Caelo	Dexamethasone	171042165585	1
Caelo	Dexamethasone	1714203	1
Caelo	Dexamethasone	173322402	1
Caelo	Dexamethasone	17332402	14
Caelo	Dexamethasone	17332403	37
Caelo	Dexamethasone	17332404	15
Caelo	Dexamethasone	17332406	8
Caelo	Dexamethasone	17332407	6
Caelo	Dexamethasone	17332408	19
Caelo	Dexamethasone	17332411	3
Caelo	Dexamethasone	17332412	10
Caelo	Dexamethasone	17332413	8
Caelo	Dexamethasone	17332414	8
Caelo	Dexamethasone	17332415	8
Caelo	Dexamethasone	17332415-D20180115Ma	1
Caelo	Dexamethasone	17332416	4
Caelo	Dexamethasone	17332417	3
Caelo	Dexamethasone	17332418	3
Caelo	Dexamethasone	17332419	26
Caelo	Dexamethasone	17e31-b01-338016	1
Caelo	Dexamethasone	1806023-01	2
Caelo	Dexamethasone	18121709	1
Caelo	Dexamethasone	190022101	1
Caelo	Dexamethasone	1902210	1
Caelo	Dexamethasone	19022101	54
Caelo	Dexamethasone	19022102	3
Caelo	Dexamethasone	19022103	9
Caelo	Dexamethasone	19022104	8
Caelo	Dexamethasone	19022107	20
Caelo	Dexamethasone	190221070	1
Caelo	Dexamethasone	19022108	5
Caelo	Dexamethasone	19022109	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dexamethasone	19022112	6
Caelo	Dexamethasone	190222112	1
Caelo	Dexamethasone	19056503	1
Caelo	Dexamethasone	190865001	16
Caelo	Dexamethasone	190865005	1
Caelo	Dexamethasone	19086501	7
Caelo	Dexamethasone	19086502	28
Caelo	Dexamethasone	19086503	53
Caelo	Dexamethasone	19086504	19
Caelo	Dexamethasone	19086508	6
Caelo	Dexamethasone	19086513	29
Caelo	Dexamethasone	190901101	1
Caelo	Dexamethasone	1909011-01	1
Caelo	Dexamethasone	19096503	1
Caelo	Dexamethasone	191072709	1
Caelo	Dexamethasone	192245004	1
Caelo	Dexamethasone	192876001	39
Caelo	Dexamethasone	192876002	1
Caelo	Dexamethasone	192876004	32
Caelo	Dexamethasone	192876005	24
Caelo	Dexamethasone	192876008	2
Caelo	Dexamethasone	192876009	14
Caelo	Dexamethasone	200002251001	2
Caelo	Dexamethasone	200002251002	1
Caelo	Dexamethasone	200002551001	1
Caelo	Dexamethasone	200003905003	1
Caelo	Dexamethasone	20002251001	26
Caelo	Dexamethasone	20002251002	11
Caelo	Dexamethasone	200039005004	1
Caelo	Dexamethasone	20003905001	3
Caelo	Dexamethasone	20003905002	16
Caelo	Dexamethasone	20003905003	19
Caelo	Dexamethasone	20003905004	11
Caelo	Dexamethasone	20003905005	21
Caelo	Dexamethasone	2000395004	2
Caelo	Dexamethasone	2005024-01	3
Caelo	Dexamethasone	2005024-02	1
Caelo	Dexamethasone	2005024-03	1
Caelo	Dexamethasone	200529SM	1
Caelo	Dexamethasone	21001380001	4
Caelo	Dexamethasone	21001380002	26
Caelo	Dexamethasone	21001380003	11
Caelo	Dexamethasone	21001380004	16
Caelo	Dexamethasone	21001380008	3
Caelo	Dexamethasone	21001380009	11
Caelo	Dexamethasone	21001380009I	1
Caelo	Dexamethasone	21001380010	13
Caelo	Dexamethasone	21001380011	7
Caelo	Dexamethasone	2100138003	1
Caelo	Dexamethasone	2100138009	3
Caelo	Dexamethasone	2100138009x2	2
Caelo	Dexamethasone	2109019-01	1
Caelo	Dexamethasone	2109019-02	1
Caelo	Dexamethasone	22000019003	1
Caelo	Dexamethasone	22000049002	1
Caelo	Dexamethasone	22000049003	12
Caelo	Dexamethasone	22000049004	7
Caelo	Dexamethasone	22000049005	6
Caelo	Dexamethasone	22000049009	1
Caelo	Dexamethasone	22000049010	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dexamethasone	22000049011	5
Caelo	Dexamethasone	2200049003	1
Caelo	Dexamethasone	2200049004	1
Caelo	Dexamethasone	2200049009	1
Caelo	Dexamethasone	22002762001	1
Caelo	Dexamethasone	22002762002	1
Caelo	Dexamethasone	22002762003	14
Caelo	Dexamethasone	22002762004	5
Caelo	Dexamethasone	22002762005	2
Caelo	Dexamethasone	22002762008	2
Caelo	Dexamethasone	22002762009	1
Caelo	Dexamethasone	22002762010	1
Caelo	Dexamethasone	22002762014	1
Caelo	Dexamethasone	22002762017	2
Caelo	Dexamethasone	2884	1
Caelo	Dexamethasone	3084310	1
Caelo	Dexamethasone	6(19086504)	1
Caelo	Dexamethasone	9383631	1
Caesar & Loretz GmbH...	Dexamethasone	22000049005	1
Caesar & Loretz GmbH...	Dexamethasone	17104211	2
Caesar & Loretz GmbH...	Dexamethasone	19022107	1
Caesar & Loretz GmbH...	Dexamethasone	22002762004	1
Caesar & Loretz GmbH...	Dexamethasone	17332416	1
Caesar & Loretz GmbH...	Dexamethasone	17332419	2
Caesar & Loretz GmbH...	Dexamethasone	19086513	1
Caesar & Loretz GmbH...	Dexamethasone	10369922	1
Caesar & Loretz GmbH/ AHD	Dexamethasone	192876005	1
Caesar & Loretz GmbH...	Dexamethasone	20002251001	1
Caesar & Loretz GmbH...	Dexamethasone	19022101	1
Caesar & Loretz GmbH...	Dexamethasone	192876004	2
Caesar & Loretz GmbH...	Dexamethasone	192876005	1
Caesar & Loretz GmbH...	Dexamethasone	20002251002	1
Caesar & Loretz GmbH...	Dexamethasone	21001380002	2
Caesar & Loretz GmbH...	Dexamethasone	20003905004	1
Caesar & Loretz GmbH...	Dexamethasone	20003905002	1
Caesar & Loretz GmbH...	Dexamethasone	22002762004	1
Caesar & Loretz GmbH...	Dexamethasone	21001380004	1
Caesar & Loretz GmbH/AHD	Dexamethasone	19086502	1
Caesar & Loretz GmbH/AHD	Dexamethasone	22000049005	1
Caesar & Loretz GmbH...	Dexamethasone	19086504	1
Caesar & Loretz GmbH...	Dexamethasone	19086513	1
Caesar & Loretz GmbH/GEHE	Dexamethasone	19086508	1
Caesar & Loretz GmbH/GEHE	Dexamethasone	192876004	2
Caesar & Loretz GmbH/Gehe	Dexamethasone	20003905002	1
Caesar & Loretz GmbH/Gehe	Dexamethasone	20003905003	1
Caesar & Loretz GmbH/GEHE	Dexamethasone	20003905003	1
Caesar & Loretz GmbH/Gehe	Dexamethasone	21001380009	1
Caesar & Loretz GmbH...	Dexamethasone	19022103	1
Caesar & Loretz GmbH...	Dexamethasone	192876005	1
Caesar & Loretz GmbH...	Dexamethasone	20003905004	1
Caesar & Loretz GmbH...	Dexamethasone	22000049004	1
Caesar & Loretz GmbH...	Dexamethasone	22002762009	1
Caesar & Loretz GmbH/Gö	Dexamethasone	192876004	1
Caesar & Loretz GmbH...	Dexamethasone	21001380009	1
Caesar & Loretz GmbH...	Dexamethasone	22000049005	1
Caesar & Loretz GmbH...	Dexamethasone	1806023-02	1
Caesar & Loretz GmbH...	Dexamethasone	19022103	1
Caesar & Loretz GmbH...	Dexamethasone	192876004	1
Caesar & Loretz GmbH...	Dexamethasone	20002251002	1
Caesar & Loretz GmbH...	Dexamethasone	21001380002	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Kehr	Dexamethasone	20003905003	1
Caesar & Loretz GmbH/Kehr	Dexamethasone	22000049003	1
Caesar & Loretz GmbH/Krie	Dexamethasone	19086503	1
Caesar & Loretz GmbH...	Dexamethasone	19086502	1
Caesar & Loretz GmbH...	Dexamethasone	192876005	1
Caesar & Loretz GmbH...	Dexamethasone	20003905003	1
Caesar & Loretz GmbH...	Dexamethasone	19086503	1
Caesar & Loretz GmbH...	Dexamethasone	192876009	1
Caesar & Loretz GmbH...	Dexamethasone	20003905003	1
Caesar & Loretz GmbH...	Dexamethasone	22000049011	1
Caesar & Loretz GmbH/Ph	Dexamethasone	21001380010	1
Caesar & Loretz GmbH/Pho	Dexamethasone	20003905003	1
Caesar & Loretz GmbH...	Dexamethasone	20003905003	1
Caesar & Loretz GmbH...	Dexamethasone	19022112	1
Caesar & Loretz GmbH...	Dexamethasone	19086502	1
Caesar & Loretz GmbH...	Dexamethasone	19086503	1
Caesar & Loretz GmbH...	Dexamethasone	19086508	1
Caesar & Loretz GmbH...	Dexamethasone	21001380002	1
Caesar & Loretz GmbH...	Dexamethasone	21001380003	1
Caesar & Loretz GmbH...	Dexamethasone	21001380004	2
Caesar & Loretz GmbH/Sa	Dexamethasone	192876004	2
Caesar & Loretz GmbH...	Dexamethasone	1909011-01	1
Caesar & Loretz GmbH...	Dexamethasone	192876009	1
Caesar & Loretz GmbH...	Dexamethasone	20002251002	1
Caesar & Loretz GmbH	Dexamethasone	15054622	1
Caesar & Loretz GmbH	Dexamethasone	161100102	1
Caesar & Loretz GmbH	Dexamethasone	17332408	1
Caesar & Loretz GmbH	Dexamethasone	17332414	1
Caesar & Loretz GmbH	Dexamethasone	17332415	1
Caesar & Loretz GmbH	Dexamethasone	17332419	1
Caesar & Loretz GmbH	Dexamethasone	19022101	9
Caesar & Loretz GmbH	Dexamethasone	19022103	1
Caesar & Loretz GmbH	Dexamethasone	19022104	1
Caesar & Loretz GmbH	Dexamethasone	19022107	7
Caesar & Loretz GmbH	Dexamethasone	19022108	1
Caesar & Loretz GmbH	Dexamethasone	190865001	2
Caesar & Loretz GmbH	Dexamethasone	19086502	10
Caesar & Loretz GmbH	Dexamethasone	19086503	6
Caesar & Loretz GmbH	Dexamethasone	19086504	7
Caesar & Loretz GmbH	Dexamethasone	19086513	3
Caesar & Loretz GmbH	Dexamethasone	1909011-01	1
Caesar & Loretz GmbH	Dexamethasone	192876001	11
Caesar & Loretz GmbH	Dexamethasone	192876002	1
Caesar & Loretz GmbH	Dexamethasone	192876004	12
Caesar & Loretz GmbH	Dexamethasone	192876005	3
Caesar & Loretz GmbH	Dexamethasone	192876008	1
Caesar & Loretz GmbH	Dexamethasone	192876009	6
Caesar & Loretz GmbH	Dexamethasone	20002251001	10
Caesar & Loretz GmbH	Dexamethasone	20002251002	4
Caesar & Loretz GmbH	Dexamethasone	20003905001	1
Caesar & Loretz GmbH	Dexamethasone	20003905002	10
Caesar & Loretz GmbH	Dexamethasone	20003905003	6
Caesar & Loretz GmbH	Dexamethasone	20003905004	5
Caesar & Loretz GmbH	Dexamethasone	20003905005	6
Caesar & Loretz GmbH	Dexamethasone	21001380002	14
Caesar & Loretz GmbH	Dexamethasone	21001380003	3
Caesar & Loretz GmbH	Dexamethasone	21001380004	5
Caesar & Loretz GmbH	Dexamethasone	21001380008	1
Caesar & Loretz GmbH	Dexamethasone	21001380009	11
Caesar & Loretz GmbH	Dexamethasone	21001380010	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Dexamethasone	21001380011	3
Caesar & Loretz GmbH	Dexamethasone	22000049003	1
Caesar & Loretz GmbH	Dexamethasone	22000049004	2
Caesar & Loretz GmbH	Dexamethasone	22000049005	4
Caesar & Loretz GmbH	Dexamethasone	22000049009	3
Caesar & Loretz GmbH	Dexamethasone	22000049010	1
Caesar & Loretz GmbH	Dexamethasone	22000049011	2
Caesar & Loretz GmbH	Dexamethasone	22002762004	4
Caesar & Loretz GmbH	Dexamethasone	22002762005	3
Caesar & Loretz GmbH	Dexamethasone	22002762009	1
Caesar & Loretz GmbH	Dexamethasone	22002762014	1
Caesar & Loretz Hilden	Dexamethasone	17332419	1
Caesar & Loretz Hilden	Dexamethasone	19086503	1
Caesar & Loretz Hilden	Dexamethasone	192876001	2
Caesar & Loretz Hilden	Dexamethasone	20003905005	1
Caesar & Loretz/AHD	Dexamethasone	19086503	1
Caesar & Loretz/Noweda	Dexamethasone	13084319	1
Caesar & Loretz/Noweda	Dexamethasone	20002251001	1
Caesar & Loretz	Dexamethasone	21001380009	1
Caesar / Gehe	Dexamethasone	17332403	1
Caesar& Loretz/Geile...	Dexamethasone	19022104	1
caesar&loretz GmbH,P...	Dexamethasone	15054622	3
Caesar&Loretz GmbH,P...	Dexamethasone	15054606	2
Caesar&Loretz GmbH/Gehe	Dexamethasone	19022101	2
Caesar&Loretz GmbH	Dexamethasone	20002251002	1
Caesar&Loretz GmbH	Dexamethasone	20003905005	1
Caesar&Loretz GmbH	Dexamethasone	22000049003	1
Caesar/Gehe	Dexamethasone	190865001	2
caesar	Dexamethasone	15054617	1
Caleo / Phoenix	Dexamethasone	20003905002	2
Caleo	Dexamethasone	15054602	2
calo	Dexamethasone	17332403	1
Cealo	Dexamethasone	17332404	1
Ebert & Jacobi	Dexamethasone	1303007-03	1
Ebert & Jacobi	Dexamethasone	1611001-01	3
Ebert&Jacobi	Dexamethasone	1601052-01	1
Ebert-Jacobi	Dexamethasone	1611001-01	1
EuRho / Phoenix	Dexamethasone	1303007-03	1
EuRho / Phoenix	Dexamethasone	15054631	1
EuRho / Phönix	Dexamethasone	2109019-01	1
EuRho Anzag	Dexamethasone	1601052-02	1
EuRho Gehe	Dexamethasone	1909011-02	1
EuRho/ Gehe	Dexamethasone	1708004-01	1
EuRho/ Noweda	Dexamethasone	2109019-02	1
EuRho/Gehe	Dexamethasone	1806023-01	1
EuRho/Noweda	Dexamethasone	17008004-01	1
EuRho/Noweda	Dexamethasone	1806023-01	1
EuRho/Noweda	Dexamethasone	1806023-03	1
EuRho/Noweda	Dexamethasone	1909011-02	1
EuRho/Phoenix	Dexamethasone	1909011-02	1
EuRho/Sanacorp	Dexamethasone	2005024-02	1
EuRho	Dexamethasone	1708004-01	1
EuRho	Dexamethasone	1806023_04	1
EuRho	Dexamethasone	1806023-01	1
EuRho	Dexamethasone	1909011-01	1
EuRho	Dexamethasone	1909011-02	2
eurho	Dexamethasone	2005024-01	1
EuRho	Dexamethasone	2005024-01	3
EuRho	Dexamethasone	2005024-02	1
EuRho	Dexamethasone	2005024-03	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho	Dexamethasone	2109019-01	1
EuRho	Dexamethasone	NUD180601	1
Eurho-Pharma	Dexamethasone	1909011-02	1
Euro OTC	Dexamethasone		4
Euro OTC	Dexamethasone	1107006-01	1
Euro OTC	Dexamethasone	111105501	1
Euro OTC	Dexamethasone	1111055-01	5
Euro OTC	Dexamethasone	1111055-02	2
Euro OTC	Dexamethasone	1200008-01	1
Euro OTC	Dexamethasone	1203032-01	4
Euro OTC	Dexamethasone	1203032-02	3
Euro OTC	Dexamethasone	1209008-01	11
Euro OTC	Dexamethasone	120900802	2
Euro OTC	Dexamethasone	1209008-02	26
Euro OTC	Dexamethasone	13030007	1
Euro OTC	Dexamethasone	13030007-01	1
Euro OTC	Dexamethasone	1303007	1
Euro OTC	Dexamethasone	130300701	4
Euro OTC	Dexamethasone	1303007-01	34
Euro OTC	Dexamethasone	130300702	2
Euro OTC	Dexamethasone	1303007-02	10
Euro OTC	Dexamethasone	130300703	2
Euro OTC	Dexamethasone	1303007-03	27
Euro OTC	Dexamethasone	1303007-04	2
Euro OTC	Dexamethasone	13352309	1
Euro OTC	Dexamethasone	14D11-B01-294031	1
Euro OTC	Dexamethasone	15054621	1
Euro OTC	Dexamethasone	1512211327	1
Euro OTC	Dexamethasone	160105201	2
Euro OTC	Dexamethasone	1601052-01	27
Euro OTC	Dexamethasone	160105202	1
Euro OTC	Dexamethasone	1601052-02	37
Euro OTC	Dexamethasone	1601052-21	1
Euro OTC	Dexamethasone	1611001	2
Euro OTC	Dexamethasone	161100101	5
Euro OTC	Dexamethasone	1611001-01	58
Euro OTC	Dexamethasone	1611001-02	2
Euro OTC	Dexamethasone	161101-01	1
Euro OTC	Dexamethasone	1702004-01	1
Euro OTC	Dexamethasone	17080004-01	1
Euro OTC	Dexamethasone	1708004	1
Euro OTC	Dexamethasone	170800401	2
Euro OTC	Dexamethasone	1708004-01	89
Euro OTC	Dexamethasone	1708004-02	6
Euro OTC	Dexamethasone	1708804-01	1
Euro OTC	Dexamethasone	17104203	1
Euro OTC	Dexamethasone	17104204	1
Euro OTC	Dexamethasone	17104210	1
Euro OTC	Dexamethasone	17104211	1
Euro OTC	Dexamethasone	17332403	1
Euro OTC	Dexamethasone	180208D/1611001-01	1
Euro OTC	Dexamethasone	1806023	2
Euro OTC	Dexamethasone	1806023_03	1
Euro OTC	Dexamethasone	180602301	2
Euro OTC	Dexamethasone	1806023-01	59
Euro OTC	Dexamethasone	1806023-010	1
Euro OTC	Dexamethasone	180602302	2
Euro OTC	Dexamethasone	1806023-02	18
Euro OTC	Dexamethasone	1806023-03	7
Euro OTC	Dexamethasone	1806023-04	19

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Dexamethasone	1806023-24	1
Euro OTC	Dexamethasone	1806032-02	1
Euro OTC	Dexamethasone	19022103	1
Euro OTC	Dexamethasone	1905014-01	1
Euro OTC	Dexamethasone	190701	1
Euro OTC	Dexamethasone	19086503	1
Euro OTC	Dexamethasone	1909011	3
Euro OTC	Dexamethasone	190901101	2
Euro OTC	Dexamethasone	1909011-01	46
Euro OTC	Dexamethasone	190901102	1
Euro OTC	Dexamethasone	1909011-02	33
Euro OTC	Dexamethasone	1909011-02P200622-1	1
Euro OTC	Dexamethasone	19909011-02	1
Euro OTC	Dexamethasone	20005024-01	1
Euro OTC	Dexamethasone	2002024-01	2
Euro OTC	Dexamethasone	2005021-03	1
Euro OTC	Dexamethasone	2005024	1
Euro OTC	Dexamethasone	2005024_04	1
Euro OTC	Dexamethasone	200502401	1
Euro OTC	Dexamethasone	2005024-01	59
Euro OTC	Dexamethasone	200502402	1
Euro OTC	Dexamethasone	2005024-02	31
Euro OTC	Dexamethasone	200502403	2
Euro OTC	Dexamethasone	2005024-03	37
Euro OTC	Dexamethasone	2005024-04	5
Euro OTC	Dexamethasone	21001215017	1
Euro OTC	Dexamethasone	21009019-01	1
Euro OTC	Dexamethasone	2109012-01	1
Euro OTC	Dexamethasone	210901901	1
Euro OTC	Dexamethasone	2109019-01	32
Euro OTC	Dexamethasone	2109019-02	11
Euro OTC	Dexamethasone	2109019-03	6
Euro OTC	Dexamethasone	2109019-0306	1
Euro OTC	Dexamethasone	21090919-01	1
Euro OTC	Dexamethasone	2208005-01	1
Euro OTC	Dexamethasone	4914501	1
Euro OTC	Dexamethasone	5213A1327	1
Euro OTC	Dexamethasone	700107	3
Euro OTC	Dexamethasone	DB003/0213	3
Euro OTC	Dexamethasone	DZ11005K	1
Euro OTC	Dexamethasone	L53613	1
Euro OTC	Dexamethasone	T45290	2
Euro RHO/Jenne	Dexamethasone	1909011-02	1
Euro Rho/Jenne	Dexamethasone	2005024-03	1
Euro/ Gehe	Dexamethasone	1909011-03	1
Euro/ Gehe	Dexamethasone	19G25-B02-363757	1
Euro/ Sanacorp	Dexamethasone	1601052-01	2
Euro/Gehe	Dexamethasone	1611001-01	1
Euro/Gehe	Dexamethasone	1708004-01	2
Euro/Noweda	Dexamethasone	1806023-01	1
Euro/Sana	Dexamethasone	2109019-01	1
EuRoh/Fiebig	Dexamethasone	1806023-01	1
EuRoh/Gehe	Dexamethasone	1806023	1
Fagron	Dexamethasone	11D26-N10	3
Fagron	Dexamethasone	11F30-N02	1
Fagron	Dexamethasone	11L08-N01	4
Fagron	Dexamethasone	1209008-01	1
Fagron	Dexamethasone	12A24-B01-35964	1
Fagron	Dexamethasone	12B06-N12	2
Fagron	Dexamethasone	12D26-N09	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Dexamethasone	12H21-N11	2
Fagron	Dexamethasone	1303007-03	1
Fagron	Dexamethasone	13D12-N09	3
Fagron	Dexamethasone	13D12-N19	1
Fagron	Dexamethasone	13G08-N13	3
Fagron	Dexamethasone	13L30-B34-289691	2
Fagron	Dexamethasone	14A22-B03	2
Fagron	Dexamethasone	14A22-B03-290700	1
Fagron	Dexamethasone	14A22-B03-290701	1
Fagron	Dexamethasone	14A22-B03-294030	1
Fagron	Dexamethasone	14D11-B01-294031	2
Fagron	Dexamethasone	14D11-B01-294032	1
Fagron	Dexamethasone	15/04-B04-315528	1
Fagron	Dexamethasone	15054603	1
Fagron	Dexamethasone	15054614	1
Fagron	Dexamethasone	15A05-B01	1
Fagron	Dexamethasone	15A05-B01-034636	1
Fagron	Dexamethasone	15a05-b01-304636	1
Fagron	Dexamethasone	15A05-B01-304636	3
Fagron	Dexamethasone	15a05-b01-304637	1
Fagron	Dexamethasone	15A05-B01-304637	1
Fagron	Dexamethasone	15C16-B07	1
Fagron	Dexamethasone	15C16-B07-308252	1
Fagron	Dexamethasone	15I04-B04-315528	2
Fagron	Dexamethasone	15K17-B07-321457	3
Fagron	Dexamethasone	16/06-B03-327323	1
Fagron	Dexamethasone	1601052-01	1
Fagron	Dexamethasone	16I06-B03-327323	3
Fagron	Dexamethasone	16I06-B03-327488	3
Fagron	Dexamethasone	16K24B05330281	1
Fagron	Dexamethasone	16K24-B05-330281	1
Fagron	Dexamethasone	1708004-01	2
Fagron	Dexamethasone	17104203	1
Fagron	Dexamethasone	17332414	1
Fagron	Dexamethasone	17C13-B07-332461	5
Fagron	Dexamethasone	17E31-B01-331860	1
Fagron	Dexamethasone	17E31-B01-338016	1
Fagron	Dexamethasone	17E31B01338017	1
Fagron	Dexamethasone	17L19-B03	1
Fagron	Dexamethasone	17L19-B03-344099	2
Fagron	Dexamethasone	17L19B03-344100	1
Fagron	Dexamethasone	17L19-B03-344100	2
Fagron	Dexamethasone	17L19-B03-344396	1
Fagron	Dexamethasone	18D09-B06	1
Fagron	Dexamethasone	18D09-B06-348185	3
Fagron	Dexamethasone	18E08-B05-350243	4
Fagron	Dexamethasone	18H07-B00-355632	1
Fagron	Dexamethasone	18H07-B02-355632	1
Fagron	Dexamethasone	18H07-B02-356113	1
Fagron	Dexamethasone	19A24B01	1
Fagron	Dexamethasone	19A24-B01	1
Fagron	Dexamethasone	19A24-B01-359624	4
Fagron	Dexamethasone	19A24-B01-359625	1
Fagron	Dexamethasone	19A24-B01-359626	3
Fagron	Dexamethasone	19A24-B01-361445	1
Fagron	Dexamethasone	19G25-B02-363751	3
Fagron	Dexamethasone	19G25-B02-363755	1
Fagron	Dexamethasone	2005024-01	1
Fagron	Dexamethasone	20B04-F06-369866	2
Fagron	Dexamethasone	20B04-F06-369867	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Dexamethasone	20E08-F04-370660	1
Fagron	Dexamethasone	20F19-F08	1
Fagron	Dexamethasone	20F19-F08-371577	4
Fagron	Dexamethasone	20F19-F08-371578	1
Fagron	Dexamethasone	20K05-F04-375225	2
Fagron	Dexamethasone	21C11-F03-377848	4
Fagron	Dexamethasone	21C11-F03-378501	5
Fagron	Dexamethasone	21H13-B20-216247	1
Fagron	Dexamethasone	22A17-B06-216246	5
Fagron	Dexamethasone	22B26-B06-220498	1
Fagron	Dexamethasone	2314A-01327	1
Fagron	Dexamethasone	700107-0002	1
Fagron	Dexamethasone	DZ11005K12B06-N12	1
Fagron	Dexamethasone	F03-3778408	1
Fagron	Dexamethasone	F06-3698606	2
Fagron	Dexamethasone	NUD160702	1
Fagron	Dexamethasone	NUD180601	1
Fargon/Noweda	Dexamethasone	19A24-B01	2
Fiebig	Dexamethasone	19086513	1
Fiebig	Dexamethasone	20003905002	1
Gatt-Koller	Dexamethasone	1801087	1
GEHE 12.03.2014	Dexamethasone	13084306	1
Gehe 8.04.2014	Dexamethasone	13084310	2
Gehe amax	Dexamethasone	1806023-04	1
Gehe Rostock	Dexamethasone	22002762004	1
Gehe, Tianyao pharma...	Dexamethasone	1909011-01	1
Gehe/ Euro	Dexamethasone	2005024-01	1
Gehe	Dexamethasone	1203032-02	1
Gehe	Dexamethasone	120900802	1
Gehe	Dexamethasone	13084317	1
Gehe	Dexamethasone	13D12-N09	2
Gehe	Dexamethasone	15054602	2
Gehe	Dexamethasone	15054621	1
Gehe	Dexamethasone	15054629	1
Gehe	Dexamethasone	15054631	1
Gehe	Dexamethasone	1601052-02	1
Gehe	Dexamethasone	1708004-01	2
Gehe	Dexamethasone	17104210	1
Gehe	Dexamethasone	17104212	1
Gehe	Dexamethasone	17332404	1
GEHE	Dexamethasone	17L19-B03-344099	1
Gehe	Dexamethasone	1806023-02	2
GEHE	Dexamethasone	18H07-B02	1
Gehe	Dexamethasone	19086501	1
Gehe	Dexamethasone	192876004	1
Gehe	Dexamethasone	20003905003	1
Gehe	Dexamethasone	2005024-01	1
Gehe	Dexamethasone	2005024-04	1
Gehe	Dexamethasone	2200004901	1
gehe	Dexamethasone	220800501	1
Gehe	Dexamethasone	F03-3785001	1
Geibo	Dexamethasone	22002762015	1
Geilenkirchen	Dexamethasone	17104205	1
Henry Lamotte Oils GmbH	Dexamethasone	13084304	1
Jenne	Dexamethasone	1806023-01	1
Jenne	Dexamethasone	1806023-02	1
Jenne	Dexamethasone	1909011-01	1
Jenne	Dexamethasone	20002251002	1
Jenne	Dexamethasone	2005024-03	1
Jenne	Dexamethasone	22002762008	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Jenne	Dexamethasone	22002762016	2
Kehr/Fargon	Dexamethasone	1806023-01	2
Kehr	Dexamethasone	17104205	1
Kehr	Dexamethasone	17104210	1
Kehr	Dexamethasone	19086508	1
Kehr	Dexamethasone	2109019-03	1
Kehr	Dexamethasone	22002762004	1
Krieger	Dexamethasone	17332406	1
L10	Dexamethasone	1708004-01	1
Noweda 02.12.2019	Dexamethasone	1806023-04	1
Noweda Taucha	Dexamethasone	2109019-01	2
Noweda	Dexamethasone	12033307	2
Noweda	Dexamethasone	1303007-03	1
Noweda	Dexamethasone	1708004-01	1
Noweda	Dexamethasone	1708004-02	1
Noweda	Dexamethasone	17104204	1
Noweda	Dexamethasone	1806023-01	1
Noweda	Dexamethasone	1806023-04	1
Noweda	Dexamethasone	19022101	2
Noweda	Dexamethasone	19086503	1
Noweda	Dexamethasone	1909011-01	1
Noweda	Dexamethasone	20002251001	2
Noweda	Dexamethasone	20003905002	1
Noweda	Dexamethasone	200039050022003905003	1
Noweda	Dexamethasone	20003905003	1
Noweda	Dexamethasone	200502404	1
Noweda	Dexamethasone	21001380003	1
Noweda	Dexamethasone	2109019-03	1
Noweda	Dexamethasone	22002762008	1
Noweda	Dexamethasone	22002762010	1
Noweda	Dexamethasone	22002762014	1
Noweda	Dexamethasone	2208005-01	1
PH Euro 8,0	Dexamethasone	15054610	1
Pharmacia / Gehe	Dexamethasone	M62488	1
Pharmacia&Upjohn Comp	Dexamethasone	1209008-02	1
Pharmacia&Upjohn Com…	Dexamethasone	1601052-02	1
Phoenix Goettin	Dexamethasone	117113352302	1
Phoenix	Dexamethasone	10369928	1
Phoenix	Dexamethasone	13084313	2
Phoenix	Dexamethasone	13g08n13	1
Phoenix	Dexamethasone	15I04-B04	1
Phoenix	Dexamethasone	17332406	1
Phoenix	Dexamethasone	17332416	1
Phoenix	Dexamethasone	17332419	1
Phoenix	Dexamethasone	19086503	1
Phoenix	Dexamethasone	1909011-01	2
Phoenix	Dexamethasone	20002251002	1
Phoenix	Dexamethasone	20004529003	1
Phoenix	Dexamethasone	200622506	1
Phoenix	Dexamethasone	2109019-01	1
Phoenix	Dexamethasone	22002762016	2
Phoenix	Dexamethasone	3405	1
Phönix Euro 23.6.21	Dexamethasone	2005024-03	1
Phönix Gotha	Dexamethasone	12033315	1
Phönix Gotha	Dexamethasone	13352311	1
Phönix Gotha	Dexamethasone	17332408	1
Phönix	Dexamethasone	12033314	1
PHÖNIX	Dexamethasone	15K17-B07	1
Phönix	Dexamethasone	1601052-02	3
Phönix	Dexamethasone	1708004-01	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Dexamethasone	1806023-01	1
Phönix	Dexamethasone	19022101	1
Phönix	Dexamethasone	1909011-01	1
Phönix	Dexamethasone	1909011-02	1
Phönix	Dexamethasone	192876005	1
Phönix	Dexamethasone	2005024-03	1
PHönix	Dexamethasone	2005024-03	1
phönix	Dexamethasone	21001380009	1
Phönix	Dexamethasone	22002762003	1
Phönix	Dexamethasone	22002762010	1
Raben-Apotheke Mildenau	Dexamethasone	1303007-01	2
Sanacorp	Dexamethasone	13084308	1
Sanacorp	Dexamethasone	13352309	1
Sanacorp	Dexamethasone	1601052-01	1
Sanacorp	Dexamethasone	17104211	1
Sanacorp	Dexamethasone	17332402	1
Sanacorp	Dexamethasone	2005024-01	1
Sanacorp	Dexamethasone	21001380011	1
Sanacorp	Dexamethasone	22002762004	1
Sanacorp	Dexamethasone	22002762008	1
Sanacorp	Dexamethasone	22002762009	1
Sanofi-Chimie FR/Noweda	Dexamethasone	15054606	2
Sanofi-Chimie, FR/ Noweda	Dexamethasone	12033308	1
Symbiotica/Noweda	Dexamethasone	1601052-02	1
Symbiotica	Dexamethasone	1303007-01	1
Symbiotica	Dexamethasone	1303007-03	2
Symbiotika	Dexamethasone	1303007-03	1
Tianijin Tianyao / Gehe	Dexamethasone	17332408	1
Tianjin Tianyao Pharm/AHD	Dexamethasone	1806023-01	1
Tianjin Tianyao Phar…	Dexamethasone	200502404	1
Tianjin/Noweda	Dexamethasone	NUD170802	1
Tianjin/Phoenix	Dexamethasone	NUD190701	1
Tianjin/Phoenix	Dexamethasone	NUD200402	1
unbekannt	Dexamethasone	12D26-N09	1

- 233 169 spectra from 1515 *Apo-Ident* customers from a total of 48 867 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dexamethasone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dexamethasone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	607	0	152 355
Type B	0	1518	0	200 566
Type C	0	2837	61	233 169

The substance/substance group *Dexamethasone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0115 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.6047 %)
Type C	100.0000 % (> 99.9007 %)	97.8951 % (> 97.7916 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21289	21289	0.00	170.00
21403	21403	0.00	98.20
21850	21289	16.64	170.69
22364	22364	0.00	86.51
22914	22914	0.00	91.41
23168	24504	9.73	174.49
23169	22364	7.15	86.84
24504	24504	0.00	175.60
24705	24504	9.25	174.09
25301	25301	0.00	175.93
26967	26967	0.00	177.14

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Dexamethasone acetate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20313-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dexamethasone acetate; Dexamethasoni acetas

Special notes

When selecting the *Dexamethasone acetate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Dexamethasone acetate	7	3	116

Second-stage model

For differentiation of the substance/substance group *Dexamethasone acetate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Dexamethasone acetate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prednisolon dihydrogen phosphate di…	57.51	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Dexamethasone acetate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Dexamethasone acetate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dexamethasone acetate	13260703	21301	40	1412430
Caelo	Dexamethasone acetate	13260706	21593	60	1502537
Caelo	Dexamethasone acetate	14200207	21815	60	20140807
Caelo	Dexamethasone acetate	14200207	21815SI	30	20140807
Caelo	Dexamethasone acetate	20002252	25448	40	2102142
Caelo	Dexamethasone acetate	20002252	25448SI	34	2102142
Caelo	Dexamethasone acetate	23000428	26942	40	20230907*
Caelo	Dexamethasone acetate	23000428	26942SI	40	20230907*
Euro OTC	Dexamethasone acetate	1405024-01	21614	60	20140620
Euro OTC	Dexamethasone acetate	1405024-01	21614SI	45	20140620
Euro OTC	Dexamethasone acetate	1708011	23693	40	20171002*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 489 spectra of 11 reference samples from the substance/substance group *Dexamethasone acetate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 473 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 281 spectra of 8 reference samples from the substance/substance group *Dexamethasone acetate*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Dexamethasone acetate	161066	22437	60
Caelo	Dexamethasone acetate	181730	24253	40
Caelo	Dexamethasone acetate	191192	24734	40
Caelo	Dexamethasone acetate	14200207	21815SI†	15
Caelo	Dexamethasone acetate	161066	22437SI	42
Caelo	Dexamethasone acetate	181730	24253SI	20
Caelo	Dexamethasone acetate	191192	24734SI	40
Euro OTC	Dexamethasone acetate	1708011	23693SI†	24

- 201 803 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 528 spectra from 272 *Apo-Ident* customers from 120 batches from the substance/substance group *Dexamethasone acetate*.

- Among them are spectra of independent samples from 116 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Dexamethasone acetate	20004529006	1
	Dexamethasone acetate	20004529009	1
	Dexamethasone acetate	20004529018	2
	Dexamethasone acetate	23000428005	1
AHD	Dexamethasone acetate	1405024-03	1
AHD	Dexamethasone acetate	18173002	1
Alliance	Dexamethasone acetate	20004529014	1
apomix	Dexamethasone acetate	1405024-03	1
Bombastus	Dexamethasone acetate	16106616	1
Caelo	Dexamethasone acetate	11093210	1
Caelo	Dexamethasone acetate	11093211	1
Caelo	Dexamethasone acetate	11093215	1
Caelo	Dexamethasone acetate	11093217	1
Caelo	Dexamethasone acetate	12021801	2
Caelo	Dexamethasone acetate	12021803	3
Caelo	Dexamethasone acetate	12021811	1
Caelo	Dexamethasone acetate	12021814	2
Caelo	Dexamethasone acetate	13100401	1
Caelo	Dexamethasone acetate	13100403	5
Caelo	Dexamethasone acetate	13100404	3
Caelo	Dexamethasone acetate	13100406	1
Caelo	Dexamethasone acetate	13100407	4
Caelo	Dexamethasone acetate	13100408	2
Caelo	Dexamethasone acetate	13260701	4
Caelo	Dexamethasone acetate	13260702	1
Caelo	Dexamethasone acetate	13260703	3
Caelo	Dexamethasone acetate	13260705	1
Caelo	Dexamethasone acetate	1405024-01	1
Caelo	Dexamethasone acetate	140502403	1
Caelo	Dexamethasone acetate	14200201	3
Caelo	Dexamethasone acetate	14200205	3
Caelo	Dexamethasone acetate	14200207	1
Caelo	Dexamethasone acetate	14200208	2
Caelo	Dexamethasone acetate	14379601	1
Caelo	Dexamethasone acetate	14379602	2
Caelo	Dexamethasone acetate	14379607	5
Caelo	Dexamethasone acetate	14379608	1
Caelo	Dexamethasone acetate	14379609	3
Caelo	Dexamethasone acetate	14379611	3
Caelo	Dexamethasone acetate	14379615	4
Caelo	Dexamethasone acetate	14379616	5
Caelo	Dexamethasone acetate	14379617	1
Caelo	Dexamethasone acetate	15243201	5
Caelo	Dexamethasone acetate	15243202	4
Caelo	Dexamethasone acetate	15243203	1
Caelo	Dexamethasone acetate	16106601	1
Caelo	Dexamethasone acetate	16106602	3
Caelo	Dexamethasone acetate	16106603	6
Caelo	Dexamethasone acetate	16106603/171025DM	1
Caelo	Dexamethasone acetate	16106604	2
Caelo	Dexamethasone acetate	16106607	4
Caelo	Dexamethasone acetate	16106608	5
Caelo	Dexamethasone acetate	16106609	1
Caelo	Dexamethasone acetate	16106610	2
Caelo	Dexamethasone acetate	16106611	2
Caelo	Dexamethasone acetate	16106612	2
Caelo	Dexamethasone acetate	16106613	4
Caelo	Dexamethasone acetate	16106615	2
Caelo	Dexamethasone acetate	16106616	8
Caelo	Dexamethasone acetate	161066165624	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dexamethasone acetate	16106617	6
Caelo	Dexamethasone acetate	16106619	5
Caelo	Dexamethasone acetate	1610662	1
Caelo	Dexamethasone acetate	16106622	2
Caelo	Dexamethasone acetate	16106623	1
Caelo	Dexamethasone acetate	16106624	2
Caelo	Dexamethasone acetate	1708011-01	1
Caelo	Dexamethasone acetate	18041813	1
Caelo	Dexamethasone acetate	18173001	11
Caelo	Dexamethasone acetate	18173002	12
Caelo	Dexamethasone acetate	18173004	5
Caelo	Dexamethasone acetate	18173007	3
Caelo	Dexamethasone acetate	18173008	6
Caelo	Dexamethasone acetate	18173010	1
Caelo	Dexamethasone acetate	18173011	7
Caelo	Dexamethasone acetate	18173012	12
Caelo	Dexamethasone acetate	18173014	2
Caelo	Dexamethasone acetate	1873011	1
Caelo	Dexamethasone acetate	1911201	1
Caelo	Dexamethasone acetate	19119021	1
Caelo	Dexamethasone acetate	191192001	9
Caelo	Dexamethasone acetate	191192002	8
Caelo	Dexamethasone acetate	191192003	1
Caelo	Dexamethasone acetate	191192004	7
Caelo	Dexamethasone acetate	191192005	5
Caelo	Dexamethasone acetate	19119201	9
Caelo	Dexamethasone acetate	19119202	15
Caelo	Dexamethasone acetate	19119204	4
Caelo	Dexamethasone acetate	191192040	1
Caelo	Dexamethasone acetate	191192201	1
Caelo	Dexamethasone acetate	20002252001	7
Caelo	Dexamethasone acetate	200045290008	1
Caelo	Dexamethasone acetate	20004529001	10
Caelo	Dexamethasone acetate	20004529002	9
Caelo	Dexamethasone acetate	20004529003	11
Caelo	Dexamethasone acetate	20004529006	5
Caelo	Dexamethasone acetate	20004529008	6
Caelo	Dexamethasone acetate	20004529009	1
Caelo	Dexamethasone acetate	20004529010	4
Caelo	Dexamethasone acetate	20004529012	1
Caelo	Dexamethasone acetate	20004529014	1
Caelo	Dexamethasone acetate	20004529015	2
Caelo	Dexamethasone acetate	20004529016	2
Caelo	Dexamethasone acetate	20004529017	1
Caelo	Dexamethasone acetate	20004529018	1
Caelo	Dexamethasone acetate	20004529019	1
Caelo	Dexamethasone acetate	2004529003	1
Caelo	Dexamethasone acetate	2004529017	1
Caelo	Dexamethasone acetate	211118(20004529002)	1
Caelo	Dexamethasone acetate	22/AKD2	1
Caelo	Dexamethasone acetate	3913Q-01326	1
Caelo	Dexamethasone acetate	4113I-01326	1
Caelo	Dexamethasone acetate	5/AD1	1
Caelo	Dexamethasone acetate	50(18173001)	1
Caelo	Dexamethasone acetate	8173004	1
Caesar & Loretz GmbH...	Dexamethasone acetate	18173004	1
Caesar & Loretz GmbH...	Dexamethasone acetate	18173012	2
Caesar & Loretz GmbH...	Dexamethasone acetate	18173008	1
Caesar & Loretz GmbH...	Dexamethasone acetate	18173012	1
Caesar & Loretz GmbH/Gehe	Dexamethasone acetate	20004529001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Gehe	Dexamethasone acetate	20004529009	1
Caesar & Loretz GmbH...	Dexamethasone acetate	20004529001	2
Caesar & Loretz GmbH...	Dexamethasone acetate	20004529001	1
Caesar & Loretz GmbH...	Dexamethasone acetate	18173008	1
Caesar & Loretz GmbH...	Dexamethasone acetate	19119202	1
Caesar & Loretz GmbH...	Dexamethasone acetate	20004529015	1
Caesar & Loretz GmbH...	Dexamethasone acetate	19119202	2
Caesar & Loretz GmbH...	Dexamethasone acetate	18173011	1
Caesar & Loretz GmbH...	Dexamethasone acetate	19119202	1
Caesar & Loretz GmbH	Dexamethasone acetate	18173002	1
Caesar & Loretz GmbH	Dexamethasone acetate	18173007	2
Caesar & Loretz GmbH	Dexamethasone acetate	18173008	3
Caesar & Loretz GmbH	Dexamethasone acetate	18173010	1
Caesar & Loretz GmbH	Dexamethasone acetate	18173012	6
Caesar & Loretz GmbH	Dexamethasone acetate	191192001	7
Caesar & Loretz GmbH	Dexamethasone acetate	191192002	2
Caesar & Loretz GmbH	Dexamethasone acetate	191192004	5
Caesar & Loretz GmbH	Dexamethasone acetate	191192005	1
Caesar & Loretz GmbH	Dexamethasone acetate	19119202	2
Caesar & Loretz GmbH	Dexamethasone acetate	19119203	1
Caesar & Loretz GmbH	Dexamethasone acetate	20002252001	1
Caesar & Loretz GmbH	Dexamethasone acetate	20004529001	4
Caesar & Loretz GmbH	Dexamethasone acetate	20004529002	1
Caesar & Loretz GmbH	Dexamethasone acetate	20004529003	3
Caesar & Loretz GmbH	Dexamethasone acetate	20004529006	1
Caesar & Loretz GmbH	Dexamethasone acetate	20004529008	1
CAESAR & LORETZ GMBH	Dexamethasone acetate	20004529008	1
Caesar & Loretz GmbH	Dexamethasone acetate	20004529009	1
Caesar & Loretz GmbH	Dexamethasone acetate	20004529010	2
Caesar & Loretz GmbH	Dexamethasone acetate	20004529015	4
Caesar & Loretz Hilden	Dexamethasone acetate	19119202	1
Caesar und Loretz GmbH	Dexamethasone acetate	18173011	1
ERho	Dexamethasone acetate	1405024-02	1
EuRho/Jenne	Dexamethasone acetate	1708011-02	1
EuRho/Noweda	Dexamethasone acetate	1708011-01	2
Eurho/Sanacorp	Dexamethasone acetate	1708011-01	1
EuRho	Dexamethasone acetate	1110007-01	1
Euro OTC	Dexamethasone acetate	1110007-01	3
Euro OTC	Dexamethasone acetate	1110007-02	5
Euro OTC	Dexamethasone acetate	1110007-03	1
Euro OTC	Dexamethasone acetate	1405024	1
Euro OTC	Dexamethasone acetate	1405024-01	1
Euro OTC	Dexamethasone acetate	140502402	1
Euro OTC	Dexamethasone acetate	1405024-02	9
Euro OTC	Dexamethasone acetate	140502403	1
Euro OTC	Dexamethasone acetate	1405024-03	19
Euro OTC	Dexamethasone acetate	1405024-04	2
Euro OTC	Dexamethasone acetate	1708011-01	27
Euro OTC	Dexamethasone acetate	1708011-02	6
europharma	Dexamethasone acetate	1110007-01	1
Fagron	Dexamethasone acetate	1110007	1
Fagron	Dexamethasone acetate	1110007-01	1
Fagron	Dexamethasone acetate	14200207	1
Fagron	Dexamethasone acetate	18173002	1
Gehe	Dexamethasone acetate	16106609	1
Gehe	Dexamethasone acetate	16106613	1
Gehe	Dexamethasone acetate	16106619	1
Gehe	Dexamethasone acetate	1708011-01	1
Gehe	Dexamethasone acetate	18173007	1
Gehe	Dexamethasone acetate	18173012	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
gehe	Dexamethasone acetate	19119021	1
Noweda	Dexamethasone acetate	1110007-02	1
Noweda	Dexamethasone acetate	13100406	1
Noweda	Dexamethasone acetate	1708011-02	1
Noweda	Dexamethasone acetate	18173010	1
Noweda	Dexamethasone acetate	20004529015	1
Phoenix	Dexamethasone acetate	20004529018	1
Phoenix	Dexamethasone acetate	23000428005	1
Phönix	Dexamethasone acetate		1
Phönix	Dexamethasone acetate	16106603	1
Sanacorp	Dexamethasone acetate	14379611	1
Sanacorp	Dexamethasone acetate	16106613	1
Sanacorp	Dexamethasone acetate	1708011-01	1
Sanacorp	Dexamethasone acetate	1708011-02	1
Sanacorp	Dexamethasone acetate	29994529018	1
Sanofi Chimie/ Gehe	Dexamethasone acetate	18173004	1

- 235 539 spectra from 1515 *Apo-Ident* customers from a total of 49 140 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dexamethasone acetate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dexamethasone acetate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	489	0	152 473
Type B	0	281	0	201 803
Type C	0	496	32	235 539

The substance/substance group *Dexamethasone acetate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7730 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.8648 %)
Type C	100.0000 % (> 99.9007 %)	93.9394 % (> 93.3712 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21301	21301	0.00	154.26
21593	21593	0.00	155.90
21614	21301	8.00	156.41
21815	21593	12.63	154.96
23693	23693	0.00	163.63
25448	25448	0.00	197.57
26942	26942	0.00	230.31

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Dextromethorphan hydrobromide monohydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	22318-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dextromethorphan hydrobromide monohydrate; Dextromethorphani hydrobromidum monohydricum

Special notes

When selecting the *Dextromethorphan hydrobromide monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Dextromethorphan hydrobromide monohydrate	7	3	7

Second-stage model

For differentiation of the substance/substance group *Dextromethorphan hydrobromide monohydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Dextromethorphan hydrobromide monohydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Menthol	101.80	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Dextromethorphan hydrobromide monohydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Dextromethorphan hydrobromide monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Dextromethorphan hydrobro…	15D23-B07-308849	22318	60	AR-16-FG-008487-02
Fagron	Dextromethorphan hydrobro…	15D23-B07-308849	22326	60	20150508
Fagron	Dextromethorphan hydrobro…	16A22-B03-321371	23103	40	20160205
Fagron	Dextromethorphan hydrobro…	17B28-B01-341594	23780	40	20170612
Fagron	Dextromethorphan hydrobro…	19A08-B03-363561	24949	40	20190201
Fagron	Dextromethorphan hydrobro…	21F02-B05-221069	26283	40	20210909
Fagron	Dextromethorphan hydrobro…	21F02-B05-221069	26283SI	20	20210909
Fagron	Dextromethorphan hydrobro…	23A21-B02-225362	26633	40	20230222
Fagron	Dextromethorphan hydrobro…	23E30-B01-230367	26817	40	20230616
Fagron	Dextromethorphan hydrobro…	23E30-B01-230367	26817SI	20	20230616

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 400 spectra of 10 reference samples from the substance/substance group *Dextromethorphan hydrobromide monohydrate*. These samples are listed above in the *calibration samples* section.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The reference samples come from 7 different batches.

- 152 562 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Dextromethorphan hydrobromide monohydrate*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Dextromethorphan hydrobro…	16E23-B02-329706	23593	40
Fagron	Dextromethorphan hydrobro…	18B09-B02-350261	24288	40
Fagron	Dextromethorphan hydrobro…	23L12-B03-234621	27166	40
Fagron	Dextromethorphan hydrobro…	23A21-B02-225362	26633SI†	20

- 201 944 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 19 spectra from 8 *Apo-Ident* customers from 9 batches from the substance/substance group *Dextromethorphan hydrobromide monohydrate*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Dextromethorphan hydrobro…	17B28-B01-345398	1
Fagron	Dextromethorphan hydrobro…	14H27-B04-299502	7

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Dextromethorphan hydrobro…	16A22-B03-319331	1
Fagron	Dextromethorphan hydrobro…	16A22-B03-321371	5
Fagron	Dextromethorphan hydrobro…	18809-B02-358862	1
Fagron	Dextromethorphan hydrobro…	18B09-B02-350261	1
Fagron	Dextromethorphan hydrobro…	18B09-B02-358862	1
Fagron	Dextromethorphan hydrobro…	19A08-B03-363561	1
Phoenix	Dextromethorphan hydrobro…	19A08-B03-363562	1

- 236 048 spectra from 1515 *Apo-Ident* customers from a total of 49 250 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dextromethorphan hydrobromide monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dextromethorphan hydrobromide monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	140	0	201 944
Type C	0	19	0	236 048

The substance/substance group *Dextromethorphan hydrobromide monohydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22318	22318	0.00	129.25
22326	22318	4.44	129.01
23103	22318	6.93	129.41
23780	22318	10.86	129.65
24949	22318	13.66	131.36
26283	22318	10.20	129.73
26633	22318	12.64	130.29
26817	22318	14.41	129.96

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Diclofenac sodium**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20022-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Diclofenac sodium; Diclofenacum natricum

Special notes

When selecting the *Diclofenac sodium* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Diclofenac sodium	7	8	182

Second-stage model

For differentiation of the substance/substance group *Diclofenac sodium* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Diclofenac sodium* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	140.64	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Diclofenac sodium* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Diclofenac sodium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Diclofenac sodium	12214219	20883	20	20120815
Caelo	Diclofenac sodium	13214311	21467	60	20130826
Caelo	Diclofenac sodium	13214311	21470	60	20130826
Caelo	Diclofenac sodium	163492	23037	40	20170112*
Euro OTC	Diclofenac sodium	1403013-01	21330	40	20140401
Euro OTC	Diclofenac sodium	1607016	22694	40	20160808*
Fagron	Diclofenac sodium	13E03-N02	20886	40	20130515
Fagron	Diclofenac sodium	12L28-B05	21261	40	20130123

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 340 spectra of 8 reference samples from the substance/substance group *Diclofenac sodium*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 622 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 390 spectra of 11 reference samples from the substance/substance group *Diclofenac sodium*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Diclofenac sodium	21000065	25860	50
Euro OTC	Diclofenac sodium	1711026	23872	40
Euro OTC	Diclofenac sodium	1904008	24618	40
Euro OTC	Diclofenac sodium	2009027	25416	40
Euro OTC	Diclofenac sodium	2307012	26857	30
Fagron	Diclofenac sodium	15D14-B04-307452	21979	60
Fagron	Diclofenac sodium	19L02-F02-367737	25176	40
Fagron	Diclofenac sodium	22L20-B04-230962	27167	40
Caelo	Diclofenac sodium	21000065	25860SI	10
Euro OTC	Diclofenac sodium	2307012	26857SI	20
Fagron	Diclofenac sodium	22L20-B04-230962	27167SI	20

- 201 694 spectra from a total of 4037 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 735 spectra from 336 *Apo-Ident* customers from 189 batches from the substance/substance group *Diclofenac sodium*.

- Among them are spectra of independent samples from 181 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Diclofenac sodium	2009027	2
	Diclofenac sodium	2009027-02	1
	Diclofenac sodium	2009027-05	5
	Diclofenac sodium	21129-B06-213571	1
	Diclofenac sodium	22L20-B04-230962	1
	Diclofenac sodium	23000021007	1
	Diclofenac sodium	2307012-01	1
	Diclofenac sodium	8/0206A	1
	Diclofenac sodium	80423750002	1
	Diclofenac sodium	RDS/2108/0206A	2
	Diclofenac sodium	RDS21080206A	1
AHD	Diclofenac sodium	1503014-01	1
AHD	Diclofenac sodium	15D14B04314450	1
Aliance Healthcare	Diclofenac sodium	2009027-03	1
Amoli/Phoenix	Diclofenac sodium	20J01-F09	1
Amoli/Phoenix	Diclofenac sodium	RDS/1807/0134A	1
Amoli	Diclofenac sodium	1503014-01	1
Bombastus	Diclofenac sodium	1711026-01	1
Caeli/Alliance	Diclofenac sodium	18202602	1
Caelo	Diclofenac sodium	11091201	1
Caelo	Diclofenac sodium	12214202	1
Caelo	Diclofenac sodium	12214205	1
Caelo	Diclofenac sodium	12214206	1
Caelo	Diclofenac sodium	12214219	2
Caelo	Diclofenac sodium	12L28-B05	1
Caelo	Diclofenac sodium	13214303	2
Caelo	Diclofenac sodium	13214304	1
Caelo	Diclofenac sodium	13214308	4
Caelo	Diclofenac sodium	13214309	3
Caelo	Diclofenac sodium	13214311	8
Caelo	Diclofenac sodium	13214312	2
Caelo	Diclofenac sodium	13214316	1
Caelo	Diclofenac sodium	13214317	5
Caelo	Diclofenac sodium	13214318	4
Caelo	Diclofenac sodium	140301301	1
Caelo	Diclofenac sodium	1503014-01	1
Caelo	Diclofenac sodium	15169604	7
Caelo	Diclofenac sodium	15169609	2
Caelo	Diclofenac sodium	15169613	2
Caelo	Diclofenac sodium	15169615	1
Caelo	Diclofenac sodium	15169617	1
Caelo	Diclofenac sodium	15169675	1
Caelo	Diclofenac sodium	15278501	1
Caelo	Diclofenac sodium	15278502	2
Caelo	Diclofenac sodium	15278505	2
Caelo	Diclofenac sodium	15278506	3
Caelo	Diclofenac sodium	15278507	1
Caelo	Diclofenac sodium	15K23-B03-318519	2
Caelo	Diclofenac sodium	15K23-B03-325753	2
Caelo	Diclofenac sodium	15K23-B03-325753	1
Caelo	Diclofenac sodium	16/29-B04-334699	1
Caelo	Diclofenac sodium	1607016-03	1
Caelo	Diclofenac sodium	16349207	3
Caelo	Diclofenac sodium	16349208	1
Caelo	Diclofenac sodium	1711026-01	1
Caelo	Diclofenac sodium	1711026-02	1
Caelo	Diclofenac sodium	1711026-03	1
Caelo	Diclofenac sodium	17J19-B01-345397	1
Caelo	Diclofenac sodium	17J19-B01-352716	1
Caelo	Diclofenac sodium	18039202	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Diclofenac sodium	18039203	3
Caelo	Diclofenac sodium	18039208	1
Caelo	Diclofenac sodium	18039210	4
Caelo	Diclofenac sodium	182026003	1
Caelo	Diclofenac sodium	182026004	6
Caelo	Diclofenac sodium	18202602	2
Caelo	Diclofenac sodium	18202606	1
Caelo	Diclofenac sodium	18202609	7
Caelo	Diclofenac sodium	20003803001	3
Caelo	Diclofenac sodium	20003803002	2
Caelo	Diclofenac sodium	20003803004	2
Caelo	Diclofenac sodium	2000383002	1
Caelo	Diclofenac sodium	2100005012	1
Caelo	Diclofenac sodium	21000065003	1
Caelo	Diclofenac sodium	21000065004	2
Caelo	Diclofenac sodium	21000065006	1
Caelo	Diclofenac sodium	21000065009	2
Caelo	Diclofenac sodium	2100006501	1
Caelo	Diclofenac sodium	21000065012	4
Caelo	Diclofenac sodium	21I29-B06-221805	1
Caelo	Diclofenac sodium	5081501	1
Caesar & Loretz GmbH	Diclofenac sodium	182026004	2
Caesar & Loretz GmbH	Diclofenac sodium	18202601	1
Caesar & Loretz GmbH	Diclofenac sodium	18202602	1
Caesar & Loretz GmbH	Diclofenac sodium	18202606	1
Caesar & Loretz GmbH	Diclofenac sodium	18202609	1
Caesar & Loretz GmbH	Diclofenac sodium	20003803001	3
Caesar & Loretz GmbH	Diclofenac sodium	20003803002	1
Caesar & Loretz GmbH	Diclofenac sodium	20003803004	1
Caesar & Loretz GmbH	Diclofenac sodium	21000065002	1
Caesar & Loretz GmbH	Diclofenac sodium	21000065006	1
Caesar & Loretz GmbH	Diclofenac sodium	21000065012	2
Caesar & Loretz GmbH	Diclofenac sodium	21000065013	1
Caesar & Loretz GmbH	Diclofenac sodium	21000065015	2
Cealo	Diclofenac sodium	160701601	1
Euph/Sanacorp	Diclofenac sodium	171102603	1
EuRho / Gehe	Diclofenac sodium	2009027-02	2
EuRho /Gumo	Diclofenac sodium	1711028-03	1
EuRho/Jenne	Diclofenac sodium	1(1711026-03)	1
Eurho/Noweda	Diclofenac sodium	2009027-02	1
EuRho/Sanacorp	Diclofenac sodium	1711026-02	2
EuRho/Sanacorp	Diclofenac sodium	1904008-02	1
EuRho/Sanacorp	Diclofenac sodium	2009027-01	1
EuRho/Spangro	Diclofenac sodium	1711026-02	2
EuRho	Diclofenac sodium	1206026-02	1
EuRho	Diclofenac sodium	1503014-01	1
EuRho	Diclofenac sodium	2009027-02	1
Euro OTC	Diclofenac sodium	11091404	1
Euro OTC	Diclofenac sodium	1111040-01	2
Euro OTC	Diclofenac sodium	12060250	1
Euro OTC	Diclofenac sodium	1206026	1
Euro OTC	Diclofenac sodium	1206026-01	7
Euro OTC	Diclofenac sodium	1206026-02	3
Euro OTC	Diclofenac sodium	12214220	1
Euro OTC	Diclofenac sodium	13111203	1
Euro OTC	Diclofenac sodium	140301301	1
Euro OTC	Diclofenac sodium	1403013-01	5
Euro OTC	Diclofenac sodium	1403013-02	7
Euro OTC	Diclofenac sodium	1403013-03	3
Euro OTC	Diclofenac sodium	1503014-01	14

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Diclofenac sodium	1503014-02	6
Euro OTC	Diclofenac sodium	15169606	1
Euro OTC	Diclofenac sodium	15K23-B03-321673	1
Euro OTC	Diclofenac sodium	16067016-03	1
Euro OTC	Diclofenac sodium	1607016-01	33
Euro OTC	Diclofenac sodium	1607016-02	17
Euro OTC	Diclofenac sodium	1607016-03	29
Euro OTC	Diclofenac sodium	1711023-03	1
Euro OTC	Diclofenac sodium	1711026	2
Euro OTC	Diclofenac sodium	1711026-01	17
Euro OTC	Diclofenac sodium	171102602	2
Euro OTC	Diclofenac sodium	1711026-02	17
Euro OTC	Diclofenac sodium	171102603	3
Euro OTC	Diclofenac sodium	1711026-03	41
Euro OTC	Diclofenac sodium	1711026-1	1
Euro OTC	Diclofenac sodium	17111026_01	1
Euro OTC	Diclofenac sodium	17J19-B01-350960	2
Euro OTC	Diclofenac sodium	1807016-01	1
Euro OTC	Diclofenac sodium	1904008	2
Euro OTC	Diclofenac sodium	190400801	3
Euro OTC	Diclofenac sodium	1904008-01	15
Euro OTC	Diclofenac sodium	1904008-02	30
Euro OTC	Diclofenac sodium	1904008-1	1
Euro OTC	Diclofenac sodium	194008-02	1
Euro OTC	Diclofenac sodium	19404008-01	1
Euro OTC	Diclofenac sodium	2009027	1
Euro OTC	Diclofenac sodium	2009027-01	18
Euro OTC	Diclofenac sodium	2009027-02	36
Euro OTC	Diclofenac sodium	2009027-03	8
Euro OTC	Diclofenac sodium	2009027-04	1
Euro OTC	Diclofenac sodium	2009027-05	1
Euro OTC	Diclofenac sodium	2091715	1
Euro OTC	Diclofenac sodium	21031703	1
Euro OTC	Diclofenac sodium	23051814	1
Euro OTC	Diclofenac sodium	25041403	1
Euro OTC	Diclofenac sodium	301180730-21	1
Euro OTC	Diclofenac sodium	31101802	1
Euro OTC	Diclofenac sodium	8051812	1
Euro OTC	Diclofenac sodium	AP201218-03	1
Euro OTC	Diclofenac sodium	AP210516-20	1
EURO/all	Diclofenac sodium	135796	1
Euro/Anzag	Diclofenac sodium	1607016-03	1
Euro/L10	Diclofenac sodium	1711026031904008-01	1
EURO/Noweda	Diclofenac sodium	140301301	1
Euro/Phönix	Diclofenac sodium	1711026	1
Euro/Phönix	Diclofenac sodium	2009027-02	1
Europharm/Otto	Diclofenac sodium	135796	1
EurRho/ Anzag	Diclofenac sodium	1403013-03	1
Fagron	Diclofenac sodium		1
Fagron	Diclofenac sodium	10031505	1
Fagron	Diclofenac sodium	12L28-B05-289773	2
Fagron	Diclofenac sodium	135796-0002	1
Fagron	Diclofenac sodium	13E03-N02	1
Fagron	Diclofenac sodium	14031411	1
Fagron	Diclofenac sodium	14G17-B08-0159A	1
Fagron	Diclofenac sodium	14G17B08297032	1
Fagron	Diclofenac sodium	14G17-B08-297032	6
Fagron	Diclofenac sodium	15D14-B04	1
Fagron	Diclofenac sodium	15D14-B04-307452	1
Fagron	Diclofenac sodium	15D14-B04-314450	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Diclofenac sodium	15D14-B04-315835	1
Fagron	Diclofenac sodium	15K23-B03	1
Fagron	Diclofenac sodium	15K23-B03-318519	2
Fagron	Diclofenac sodium	15K23-B03-321673	6
Fagron	Diclofenac sodium	15K23-B03-324025	6
Fagron	Diclofenac sodium	15K23-B03-325753	5
Fagron	Diclofenac sodium	15K23-B03-327802	5
Fagron	Diclofenac sodium	16/29-B04-332372	1
Fagron	Diclofenac sodium	1607016-03	3
Fagron	Diclofenac sodium	16I29-B04	1
Fagron	Diclofenac sodium	16I29-B04-332372	4
Fagron	Diclofenac sodium	16l29	1
Fagron	Diclofenac sodium	17F02	1
Fagron	Diclofenac sodium	17F02-B05	1
Fagron	Diclofenac sodium	17F02-B05-338797	8
Fagron	Diclofenac sodium	17J19-B01	1
Fagron	Diclofenac sodium	17j19-B01-342310	1
Fagron	Diclofenac sodium	17J19-B01-342310	4
Fagron	Diclofenac sodium	17J19-B01-345397	2
Fagron	Diclofenac sodium	17J19-B01-350960	3
Fagron	Diclofenac sodium	17J19-B01-352716	3
Fagron	Diclofenac sodium	17j19-b01-354796	1
Fagron	Diclofenac sodium	17j19-B01-354796	1
Fagron	Diclofenac sodium	17J19-B01-354796	2
Fagron	Diclofenac sodium	17J19-B01B350960	1
Fagron	Diclofenac sodium	18H24-B07	2
Fagron	Diclofenac sodium	18H24-B07-357416	5
Fagron	Diclofenac sodium	18H24-B07-358891	5
Fagron	Diclofenac sodium	19L02-F02	1
Fagron	Diclofenac sodium	19L02-F02-367737	4
Fagron	Diclofenac sodium	19L02-F02-368388	3
Fagron	Diclofenac sodium	19L02-F02-369055	1
Fagron	Diclofenac sodium	19LO2-FO2-367737	1
Fagron	Diclofenac sodium	20J01-F09-0043A	1
Fagron	Diclofenac sodium	20J01-F09-374507	6
Fagron	Diclofenac sodium	21129-BO6-221805	1
Fagron	Diclofenac sodium	21C26-F04-377842	3
Fagron	Diclofenac sodium	21I29-B06-221805	11
Fagron	Diclofenac sodium	314450	1
Fagron	Diclofenac sodium	5041401	1
Fagron	Diclofenac sodium	F02-3677307	1
Fagron	Diclofenac sodium	F02-367737	1
Fagron	Diclofenac sodium	F02-3683808	1
Fagron	Diclofenac sodium	f04-3778402	1
Fagron	Diclofenac sodium	F09-3745007	2
Fagron	Diclofenac sodium	RDS/1405/0159A	1
Fagron	Diclofenac sodium	RDS/1607/334699	1
Fargon GmbH & Co.KG	Diclofenac sodium	15K23-B03-325753	1
Fargron	Diclofenac sodium	14G17-B08-297032	1
FIEBIG	Diclofenac sodium	20003803002	1
Fischar/Phönix	Diclofenac sodium	13214311	1
Fragon/Sanacorp	Diclofenac sodium	19L02-F02-3699055	1
Gehe	Diclofenac sodium	1206026-01	1
Gehe	Diclofenac sodium	15278502	1
Gehe	Diclofenac sodium	1711026-03	1
GEHE	Diclofenac sodium	17J19-B01-342310	1
Gehe	Diclofenac sodium	1904008-01	2
Gehe	Diclofenac sodium	547718202609	1
Gehe	Diclofenac sodium	A22370D230	1
Geilenkirchen	Diclofenac sodium	15278502	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Hedinger/Phoenix	Diclofenac sodium	15278506	3
Hubei Gedian Humanwe…	Diclofenac sodium	1711026-02	1
JENNE	Diclofenac sodium	17J19-B01	1
Kehr	Diclofenac sodium	1711026-03	1
L11	Diclofenac sodium	15278506	1
L12	Diclofenac sodium	18039202	1
Noveda	Diclofenac sodium	30120071252	1
Noweda/EuRho	Diclofenac sodium	1904008-02	1
Noweda	Diclofenac sodium	11G12-N06	1
Noweda	Diclofenac sodium	1403013-01	1
Noweda	Diclofenac sodium	15278504	1
Noweda	Diclofenac sodium	1711026-03	1
Noweda	Diclofenac sodium	18039202	1
Noweda	Diclofenac sodium	18202602	1
Noweda	Diclofenac sodium	1904008-01	1
Noweda	Diclofenac sodium	19L02-F02-367737	1
Noweda	Diclofenac sodium	2009027-03	1
NOWEDA	Diclofenac sodium	2009027-05	1
Phoenix	Diclofenac sodium	15K23-B03	1
Phoenix	Diclofenac sodium	1711026-02	1
Phoenix	Diclofenac sodium	19L02-F02-368388	1
Phönix	Diclofenac sodium	1403013-03	1
Phönix	Diclofenac sodium	1607016-02	1
Phönix	Diclofenac sodium	1711026-03	1
PHÖNIX	Diclofenac sodium	17F02-B05	1
Phönix	Diclofenac sodium	17F02-B05-338797	1
Phönix	Diclofenac sodium	21i29-b06-213571	1
Phönix	Diclofenac sodium	F02-3677307	1
sana	Diclofenac sodium	2009027-03	1
Sanacorp	Diclofenac sodium	1206026-01	1
SANACORP	Diclofenac sodium	18039204	1
SANACORP	Diclofenac sodium	18202606	1
Sanacorp	Diclofenac sodium	2009027-03	1
Sanacorp	Diclofenac sodium	3616Q-02994	1
siehe Protokoll	Diclofenac sodium	15169617	1

- 235 332 spectra from 1515 *Apo-Ident* customers from a total of 49 069 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Diclofenac sodium* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Diclofenac sodium* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	340	0	152 622
Type B	0	390	0	201 694
Type C	0	732	3	235 332

The substance/substance group *Diclofenac sodium* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2353 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.4615 %)
Type C	100.0000 % (> 99.9007 %)	99.5918 % (> 99.1837 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20883	23037	10.93	318.45
20886	23037	24.16	326.31
21261	23037	29.34	317.54
21330	23037	18.02	326.19
21467	23037	16.43	323.16
21470	23037	6.93	329.50
22694	22694	0.00	256.71
23037	23037	0.00	321.31

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Diltiazem hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20043-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Diltiazem hydrochloride; Diltiazemi hydrochloridum

Special notes

When selecting the *Diltiazem hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Diltiazem hydrochloride	6	6	642

Second-stage model

For differentiation of the substance/substance group *Diltiazem hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Diltiazem hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cocaine hydrochloride	72.75	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Diltiazem hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Diltiazem hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Diltiazem hydrochloride	13346914	21300	40	20131028
Caelo	Diltiazem hydrochloride	13346914	21406	60	20131028
Caelo	Diltiazem hydrochloride	13346914	21407	60	20131028
Caelo	Diltiazem hydrochloride	161908	22631	40	20160715*
Caelo	Diltiazem hydrochloride	170432	23325	40	20170331*
Fagron	Diltiazem hydrochloride	14C12-B04	21270	40	20140417
Fagron	Diltiazem hydrochloride	16G20-B03-328133	23015	40	20160829
Fagron	Diltiazem hydrochloride	16G20-B03-328133	23016	40	20160829
Fagron	Diltiazem hydrochloride	20C12-F03-371907	25365	40	20200713

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 400 spectra of 9 reference samples from the substance/substance group *Diltiazem hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 562 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 300 spectra of 9 reference samples from the substance/substance group *Diltiazem hydrochloride*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Diltiazem hydrochloride	173370	23826	40
Caelo	Diltiazem hydrochloride	183011	24389	40
Caelo	Diltiazem hydrochloride	190841	24505	40
Caelo	Diltiazem hydrochloride	22001215	26115	40
Caelo	Diltiazem hydrochloride	23001896	26950	40
Fagron	Diltiazem hydrochloride	23H17-B02-238695	27376	40
Caelo	Diltiazem hydrochloride	22001215	26115SI	20
Caelo	Diltiazem hydrochloride	23001896	26950SI	20
Fagron	Diltiazem hydrochloride	23H17-B02-238695	27376SI	20

- 201 784 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4555 spectra from 1143 *Apo-Ident* customers from 697 batches from the substance/substance group *Diltiazem hydrochloride*.

- Among them are spectra of independent samples from 642 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Diltiazem hydrochloride	135968-0009	1
	Diltiazem hydrochloride	20C12-F03-371907	1
	Diltiazem hydrochloride	21D26-F02-378333	1
	Diltiazem hydrochloride	21F11-B03-218858	2
	Diltiazem hydrochloride	21F11-B03-221071	1
	Diltiazem hydrochloride	21F11-B03-223064	2
	Diltiazem hydrochloride	21F11-BB03-221071	1
	Diltiazem hydrochloride	21F11-Bo3-221072	1
	Diltiazem hydrochloride	22/13-B07-223063	2
	Diltiazem hydrochloride	22/13-B07225364	1
	Diltiazem hydrochloride	22001215002	1
	Diltiazem hydrochloride	22001215009	1
	Diltiazem hydrochloride	22001215011	1
	Diltiazem hydrochloride	22001215012	5
	Diltiazem hydrochloride	22001215018	2
	Diltiazem hydrochloride	22001215019	9
	Diltiazem hydrochloride	22001215024	9
	Diltiazem hydrochloride	22001215026	7
	Diltiazem hydrochloride	22001215028	1
	Diltiazem hydrochloride	22001215029	20
	Diltiazem hydrochloride	22001215030	25
	Diltiazem hydrochloride	2200121512	1
	Diltiazem hydrochloride	2201215029	1
	Diltiazem hydrochloride	22113-B07-223063	2
	Diltiazem hydrochloride	22113-B07-223065	1
	Diltiazem hydrochloride	22I13-B07-223063	12
	Diltiazem hydrochloride	22I13-B07-223065	1
	Diltiazem hydrochloride	22I13-B07-225364	8
	Diltiazem hydrochloride	22I13-B07-225365	1
	Diltiazem hydrochloride	22I13-B07-225366	2
	Diltiazem hydrochloride	22I13-BO7-223063	1
	Diltiazem hydrochloride	23001896002	2
	Diltiazem hydrochloride	23001896007	8
	Diltiazem hydrochloride	23001896008	3
	Diltiazem hydrochloride	23C20-B02-227683	7
	Diltiazem hydrochloride	23C20-B02-227685	1
	Diltiazem hydrochloride	23G06-B07-232368	1
	Diltiazem hydrochloride	23G06-B07-234623	2
	Diltiazem hydrochloride	23G06-B07-2347623	1
	Diltiazem hydrochloride	23G06-B08-236814	1
	Diltiazem hydrochloride	23H17-B02-238694	1
	Diltiazem hydrochloride	24000125005	1
	Diltiazem hydrochloride	24000125006	1
	Diltiazem hydrochloride	24000125007	1
	Diltiazem hydrochloride	Az-0350522	1
	Diltiazem hydrochloride	AZ-0350522	1
	Diltiazem hydrochloride	AZ-0440321	1
	Diltiazem hydrochloride	AZ-0951022	1
	Diltiazem hydrochloride	B02-2276803	4
	Diltiazem hydrochloride	B07-2230603	1
	Diltiazem hydrochloride	Dil17052023	1
11.08.14 Phoenix	Diltiazem hydrochloride	13346901	1
AEP	Diltiazem hydrochloride	22001215013	1
AHD	Diltiazem hydrochloride	14C12-B04-292757	1
AHD	Diltiazem hydrochloride	15G20-B08-314375	1
AHD	Diltiazem hydrochloride	17043210	1
AHD	Diltiazem hydrochloride	17337017	2
AHD	Diltiazem hydrochloride	18301108	3
AHD	Diltiazem hydrochloride	18A29-B01-345623	2
AHD	Diltiazem hydrochloride	20000622010	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
AHD	Diltiazem hydrochloride	21000035021	1
AHD	Diltiazem hydrochloride	22001215029	1
AHD	Diltiazem hydrochloride	22001215030	1
ALH	Diltiazem hydrochloride	15414319	1
Alliance Health	Diltiazem hydrochloride	13A02-N05	1
Alliance Healthcare	Diltiazem hydrochloride	12I12-N02	1
Alliance Healthcare	Diltiazem hydrochloride	22001215007	1
Alliance	Diltiazem hydrochloride	12133008	1
Alliance	Diltiazem hydrochloride	12133009	1
Alliance	Diltiazem hydrochloride	22I13-B07-223065	1
allianz	Diltiazem hydrochloride	15230512	1
Anzag	Diltiazem hydrochloride	13346915	1
anzag	Diltiazem hydrochloride	15414319	2
Anzag	Diltiazem hydrochloride	17043203	1
apomix	Diltiazem hydrochloride	14C12-B04-292759	1
Bomastus / Alliance ...	Diltiazem hydrochloride	17043219	1
Bombastus	Diltiazem hydrochloride	16190813	1
Caelo	Diltiazem hydrochloride		4
Caelo	Diltiazem hydrochloride	10069509	1
Caelo	Diltiazem hydrochloride	1020617/16190813	1
Caelo	Diltiazem hydrochloride	10212404	1
Caelo	Diltiazem hydrochloride	10212413	1
Caelo	Diltiazem hydrochloride	1090917/17043203	1
Caelo	Diltiazem hydrochloride	1091503	1
Caelo	Diltiazem hydrochloride	11091301	1
Caelo	Diltiazem hydrochloride	11134113	1
Caelo	Diltiazem hydrochloride	11134117	4
Caelo	Diltiazem hydrochloride	11L20-N06	1
Caelo	Diltiazem hydrochloride	12/12-N02	1
Caelo	Diltiazem hydrochloride	12051802	1
Caelo	Diltiazem hydrochloride	12133006	1
Caelo	Diltiazem hydrochloride	12133008	2
Caelo	Diltiazem hydrochloride	12133009	7
Caelo	Diltiazem hydrochloride	12133010	12
Caelo	Diltiazem hydrochloride	12133011	3
Caelo	Diltiazem hydrochloride	12133014	2
Caelo	Diltiazem hydrochloride	12133022	11
Caelo	Diltiazem hydrochloride	12133023	1
Caelo	Diltiazem hydrochloride	12133028	4
Caelo	Diltiazem hydrochloride	12133029	4
Caelo	Diltiazem hydrochloride	12176801	1
Caelo	Diltiazem hydrochloride	12176804	1
Caelo	Diltiazem hydrochloride	12177101	13
Caelo	Diltiazem hydrochloride	1250417	1
Caelo	Diltiazem hydrochloride	13031501	1
Caelo	Diltiazem hydrochloride	13102004	1
Caelo	Diltiazem hydrochloride	1319604	1
Caelo	Diltiazem hydrochloride	13196103	2
Caelo	Diltiazem hydrochloride	13196104	7
Caelo	Diltiazem hydrochloride	13196105	17
Caelo	Diltiazem hydrochloride	13196107	3
Caelo	Diltiazem hydrochloride	1334609	1
Caelo	Diltiazem hydrochloride	13346901	8
Caelo	Diltiazem hydrochloride	13346902	5
Caelo	Diltiazem hydrochloride	13346903	10
Caelo	Diltiazem hydrochloride	13346904	5
Caelo	Diltiazem hydrochloride	13346905	9
Caelo	Diltiazem hydrochloride	13346908	1
Caelo	Diltiazem hydrochloride	13346914	6
Caelo	Diltiazem hydrochloride	13346915	8

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Diltiazem hydrochloride	1396103	1
Caelo	Diltiazem hydrochloride	13A02-N05	1
Caelo	Diltiazem hydrochloride	13G16-N05	1
Caelo	Diltiazem hydrochloride	13G16-No5	1
Caelo	Diltiazem hydrochloride	13J24-B04-286569	1
Caelo	Diltiazem hydrochloride	13j24-b04-286571	1
Caelo	Diltiazem hydrochloride	13J24-B04-289432	3
Caelo	Diltiazem hydrochloride	1405904	1
Caelo	Diltiazem hydrochloride	14059133	1
Caelo	Diltiazem hydrochloride	140595	1
Caelo	Diltiazem hydrochloride	14059502	1
Caelo	Diltiazem hydrochloride	14059503	3
Caelo	Diltiazem hydrochloride	14059504	3
Caelo	Diltiazem hydrochloride	14059513	18
Caelo	Diltiazem hydrochloride	14059514	16
Caelo	Diltiazem hydrochloride	140595143	1
Caelo	Diltiazem hydrochloride	14059515	3
Caelo	Diltiazem hydrochloride	14059521	2
Caelo	Diltiazem hydrochloride	14318402	4
Caelo	Diltiazem hydrochloride	14318403	4
Caelo	Diltiazem hydrochloride	14318409	14
Caelo	Diltiazem hydrochloride	14318410	3
Caelo	Diltiazem hydrochloride	14318412	18
Caelo	Diltiazem hydrochloride	14318413	3
Caelo	Diltiazem hydrochloride	14318414	3
Caelo	Diltiazem hydrochloride	14318416	2
Caelo	Diltiazem hydrochloride	1459513	1
Caelo	Diltiazem hydrochloride	14C12-B04-292757	1
Caelo	Diltiazem hydrochloride	14C12-B04-294133	1
Caelo	Diltiazem hydrochloride	14C12-B04-294135	1
Caelo	Diltiazem hydrochloride	14g22b08299781	1
Caelo	Diltiazem hydrochloride	14G22-B08-299781	1
Caelo	Diltiazem hydrochloride	15/246/DI	1
Caelo	Diltiazem hydrochloride	15212801	11
Caelo	Diltiazem hydrochloride	15212802	8
Caelo	Diltiazem hydrochloride	15212806	2
Caelo	Diltiazem hydrochloride	1521806	1
Caelo	Diltiazem hydrochloride	15230000000000000000	1
Caelo	Diltiazem hydrochloride	15230501	7
Caelo	Diltiazem hydrochloride	15230502	14
Caelo	Diltiazem hydrochloride	15230503	12
Caelo	Diltiazem hydrochloride	15230504	3
Caelo	Diltiazem hydrochloride	15230507	5
Caelo	Diltiazem hydrochloride	15230510	3
Caelo	Diltiazem hydrochloride	15230512	17
Caelo	Diltiazem hydrochloride	15230513	1
Caelo	Diltiazem hydrochloride	15230514	3
Caelo	Diltiazem hydrochloride	15230515	1
Caelo	Diltiazem hydrochloride	15230516	1
Caelo	Diltiazem hydrochloride	152341904111	1
Caelo	Diltiazem hydrochloride	154114319	1
Caelo	Diltiazem hydrochloride	15414301	21
Caelo	Diltiazem hydrochloride	15414302	15
Caelo	Diltiazem hydrochloride	15414303	1
Caelo	Diltiazem hydrochloride	15414304	1
Caelo	Diltiazem hydrochloride	15414305	4
Caelo	Diltiazem hydrochloride	15414309	2
Caelo	Diltiazem hydrochloride	15414310	1
Caelo	Diltiazem hydrochloride	15414312	1
Caelo	Diltiazem hydrochloride	15414313	16

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Diltiazem hydrochloride	15414318	1
Caelo	Diltiazem hydrochloride	15414319	31
Caelo	Diltiazem hydrochloride	15414320	1
Caelo	Diltiazem hydrochloride	15414321	2
Caelo	Diltiazem hydrochloride	15435807	1
Caelo	Diltiazem hydrochloride	15B12-B01-305399	1
Caelo	Diltiazem hydrochloride	15B12-B01-305400	1
Caelo	Diltiazem hydrochloride	15B12-B01-305401	1
Caelo	Diltiazem hydrochloride	15G20B-08-312065	1
Caelo	Diltiazem hydrochloride	15G20-B08-312065	2
Caelo	Diltiazem hydrochloride	15G20-B08-314375	2
Caelo	Diltiazem hydrochloride	160415D	1
Caelo	Diltiazem hydrochloride	161908	1
Caelo	Diltiazem hydrochloride	16190801	4
Caelo	Diltiazem hydrochloride	16190805	3
Caelo	Diltiazem hydrochloride	16190806	16
Caelo	Diltiazem hydrochloride	16190807	3
Caelo	Diltiazem hydrochloride	16190810	11
Caelo	Diltiazem hydrochloride	16190813	16
Caelo	Diltiazem hydrochloride	16190814	13
Caelo	Diltiazem hydrochloride	16190815	1
Caelo	Diltiazem hydrochloride	16190817	2
Caelo	Diltiazem hydrochloride	16190818	1
Caelo	Diltiazem hydrochloride	16A18-B07-31667	1
Caelo	Diltiazem hydrochloride	16A18-B07-318732	2
Caelo	Diltiazem hydrochloride	16A18-B07-318733	1
Caelo	Diltiazem hydrochloride	16A18-B07-319570	1
Caelo	Diltiazem hydrochloride	16C14_B11_322642	1
Caelo	Diltiazem hydrochloride	16C14-B11-320849	1
Caelo	Diltiazem hydrochloride	16C14-B11-322153	2
Caelo	Diltiazem hydrochloride	16G20_B03_325903	1
Caelo	Diltiazem hydrochloride	16G20-B03-325903	3
Caelo	Diltiazem hydrochloride	16G20-B03-328133	2
Caelo	Diltiazem hydrochloride	16L19-B01-330365	3
Caelo	Diltiazem hydrochloride	170043217	1
Caelo	Diltiazem hydrochloride	1704317	1
Caelo	Diltiazem hydrochloride	170432	1
Caelo	Diltiazem hydrochloride	17043202	27
Caelo	Diltiazem hydrochloride	17043203	15
Caelo	Diltiazem hydrochloride	17043204	13
Caelo	Diltiazem hydrochloride	17043205	9
Caelo	Diltiazem hydrochloride	17043207	1
Caelo	Diltiazem hydrochloride	17043208	1
Caelo	Diltiazem hydrochloride	17043210	2
Caelo	Diltiazem hydrochloride	17043212	1
Caelo	Diltiazem hydrochloride	17043213	2
Caelo	Diltiazem hydrochloride	17043215	21
Caelo	Diltiazem hydrochloride	17043216	32
Caelo	Diltiazem hydrochloride	17043217	30
Caelo	Diltiazem hydrochloride	17043218	20
Caelo	Diltiazem hydrochloride	17043219	29
Caelo	Diltiazem hydrochloride	17043223	9
Caelo	Diltiazem hydrochloride	17043224	9
Caelo	Diltiazem hydrochloride	17043227	1
Caelo	Diltiazem hydrochloride	17043228	5
Caelo	Diltiazem hydrochloride	17043230	5
Caelo	Diltiazem hydrochloride	17053181	1
Caelo	Diltiazem hydrochloride	170602DH/16190813	1
Caelo	Diltiazem hydrochloride	170729181	1
Caelo	Diltiazem hydrochloride	17331012	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Diltiazem hydrochloride	17332021	1
Caelo	Diltiazem hydrochloride	173327027	1
Caelo	Diltiazem hydrochloride	173337018	1
Caelo	Diltiazem hydrochloride	173337026	1
Caelo	Diltiazem hydrochloride	17337004	14
Caelo	Diltiazem hydrochloride	17337005	33
Caelo	Diltiazem hydrochloride	17337007	2
Caelo	Diltiazem hydrochloride	17337009	49
Caelo	Diltiazem hydrochloride	1733701	1
Caelo	Diltiazem hydrochloride	17337010	9
Caelo	Diltiazem hydrochloride	17337011	16
Caelo	Diltiazem hydrochloride	17337012	23
Caelo	Diltiazem hydrochloride	17337014	14
Caelo	Diltiazem hydrochloride	17337016	10
Caelo	Diltiazem hydrochloride	17337017	3
Caelo	Diltiazem hydrochloride	17337018	39
Caelo	Diltiazem hydrochloride	17337025	26
Caelo	Diltiazem hydrochloride	17337026	43
Caelo	Diltiazem hydrochloride	17337027	31
Caelo	Diltiazem hydrochloride	1733712	1
Caelo	Diltiazem hydrochloride	17D11-B11-333704	1
Caelo	Diltiazem hydrochloride	17D11-B11-333705	2
Caelo	Diltiazem hydrochloride	17D11-B11-334192	3
Caelo	Diltiazem hydrochloride	17D11-B11-334837	3
Caelo	Diltiazem hydrochloride	17H25-B01-340697	2
Caelo	Diltiazem hydrochloride	17h25-b01340699	1
Caelo	Diltiazem hydrochloride	17H25-B01-343273	1
Caelo	Diltiazem hydrochloride	180320DHC/17043218	1
Caelo	Diltiazem hydrochloride	18041802	1
Caelo	Diltiazem hydrochloride	18061511	1
Caelo	Diltiazem hydrochloride	18259501	1
Caelo	Diltiazem hydrochloride	18301108	1
Caelo	Diltiazem hydrochloride	18301109	8
Caelo	Diltiazem hydrochloride	1830111	1
Caelo	Diltiazem hydrochloride	18301110	13
Caelo	Diltiazem hydrochloride	18301111	37
Caelo	Diltiazem hydrochloride	1831110	1
Caelo	Diltiazem hydrochloride	18A29_B01_345623	1
Caelo	Diltiazem hydrochloride	18A29-B01	2
Caelo	Diltiazem hydrochloride	18A29-B01-345624	1
Caelo	Diltiazem hydrochloride	18a29-b01-347886	1
Caelo	Diltiazem hydrochloride	18A29-B01-348861	4
Caelo	Diltiazem hydrochloride	18A29-B01-352907	1
Caelo	Diltiazem hydrochloride	18A29-B01-352909	1
Caelo	Diltiazem hydrochloride	18A29-BO1-348861	1
Caelo	Diltiazem hydrochloride	18H09-B03	2
Caelo	Diltiazem hydrochloride	18H09-B03-352908	1
Caelo	Diltiazem hydrochloride	18H09-B03-358917	4
Caelo	Diltiazem hydrochloride	18H09-B03-358918	1
Caelo	Diltiazem hydrochloride	18H09-B03-362596	2
Caelo	Diltiazem hydrochloride	18H09-B03-366217	1
Caelo	Diltiazem hydrochloride	18H09-B03-366218	1
Caelo	Diltiazem hydrochloride	18h09-b03-366219	1
Caelo	Diltiazem hydrochloride	1904108	1
Caelo	Diltiazem hydrochloride	190840108	1
Caelo	Diltiazem hydrochloride	190841002	9
Caelo	Diltiazem hydrochloride	190841004	3
Caelo	Diltiazem hydrochloride	190841005	25
Caelo	Diltiazem hydrochloride	190841006	33
Caelo	Diltiazem hydrochloride	190841007	30

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Diltiazem hydrochloride	19084103	7
Caelo	Diltiazem hydrochloride	19084104	17
Caelo	Diltiazem hydrochloride	19084105	32
Caelo	Diltiazem hydrochloride	19084106	39
Caelo	Diltiazem hydrochloride	19084107	29
Caelo	Diltiazem hydrochloride	19084108	40
Caelo	Diltiazem hydrochloride	19084110	21
Caelo	Diltiazem hydrochloride	19084110P-191028-1	1
Caelo	Diltiazem hydrochloride	19084110P-200217-2	1
Caelo	Diltiazem hydrochloride	19084111	13
Caelo	Diltiazem hydrochloride	19084115	22
Caelo	Diltiazem hydrochloride	190941007/3720	1
Caelo	Diltiazem hydrochloride	19841006	1
Caelo	Diltiazem hydrochloride	19H09-B03-366217	1
Caelo	Diltiazem hydrochloride	20000622003	16
Caelo	Diltiazem hydrochloride	20000622007	2
Caelo	Diltiazem hydrochloride	20000622008	8
Caelo	Diltiazem hydrochloride	20000622009	16
Caelo	Diltiazem hydrochloride	20000622010	37
Caelo	Diltiazem hydrochloride	20000622011	21
Caelo	Diltiazem hydrochloride	20000622014	2
Caelo	Diltiazem hydrochloride	20000622015	14
Caelo	Diltiazem hydrochloride	2000622011	1
Caelo	Diltiazem hydrochloride	2000622015	1
Caelo	Diltiazem hydrochloride	20C12-F03-371907	1
Caelo	Diltiazem hydrochloride	20C-12-F03-371907	1
Caelo	Diltiazem hydrochloride	20J01F11374760	1
Caelo	Diltiazem hydrochloride	20J01-F11-374763	1
Caelo	Diltiazem hydrochloride	210000035001	1
Caelo	Diltiazem hydrochloride	210000035012	1
Caelo	Diltiazem hydrochloride	21000035001	21
Caelo	Diltiazem hydrochloride	21000035002	30
Caelo	Diltiazem hydrochloride	21000035003	30
Caelo	Diltiazem hydrochloride	21000035004	3
Caelo	Diltiazem hydrochloride	210000350069	1
Caelo	Diltiazem hydrochloride	21000035008	8
Caelo	Diltiazem hydrochloride	21000035009	29
Caelo	Diltiazem hydrochloride	21000035010	29
Caelo	Diltiazem hydrochloride	21000035011	16
Caelo	Diltiazem hydrochloride	21000035012	18
Caelo	Diltiazem hydrochloride	21000035013	3
Caelo	Diltiazem hydrochloride	21000035016	10
Caelo	Diltiazem hydrochloride	21000035017	25
Caelo	Diltiazem hydrochloride	21000035021	9
Caelo	Diltiazem hydrochloride	21000035023	2
Caelo	Diltiazem hydrochloride	2100003509	1
Caelo	Diltiazem hydrochloride	2100003510	1
Caelo	Diltiazem hydrochloride	21000035100	1
Caelo	Diltiazem hydrochloride	21000035101	1
Caelo	Diltiazem hydrochloride	2100003517	1
Caelo	Diltiazem hydrochloride	2100003521	1
Caelo	Diltiazem hydrochloride	2100035003	2
Caelo	Diltiazem hydrochloride	2100035010	1
Caelo	Diltiazem hydrochloride	2100035017	1
Caelo	Diltiazem hydrochloride	2100035021	2
Caelo	Diltiazem hydrochloride	21D26-F02-378333	3
Caelo	Diltiazem hydrochloride	21F11-B03-221071	1
Caelo	Diltiazem hydrochloride	22000062009	1
Caelo	Diltiazem hydrochloride	22001215001	1
Caelo	Diltiazem hydrochloride	22001215003	24

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Diltiazem hydrochloride	22001215007	11
Caelo	Diltiazem hydrochloride	22001215008	19
Caelo	Diltiazem hydrochloride	22001215009	13
Caelo	Diltiazem hydrochloride	22001215011	5
Caelo	Diltiazem hydrochloride	22001215012	7
Caelo	Diltiazem hydrochloride	22001215013	5
Caelo	Diltiazem hydrochloride	22001215015	9
Caelo	Diltiazem hydrochloride	22001215019	5
Caelo	Diltiazem hydrochloride	22001215026	1
Caelo	Diltiazem hydrochloride	22001215029	1
Caelo	Diltiazem hydrochloride	22001215030	1
Caelo	Diltiazem hydrochloride	2200125007	1
Caelo	Diltiazem hydrochloride	2200125015	1
Caelo	Diltiazem hydrochloride	2201215008	1
Caelo	Diltiazem hydrochloride	221001215008	1
Caelo	Diltiazem hydrochloride	22L13-B07-223063	1
Caelo	Diltiazem hydrochloride	23051818	1
Caelo	Diltiazem hydrochloride	2310213562	1
Caelo	Diltiazem hydrochloride	23121402	1
Caelo	Diltiazem hydrochloride	24061706	1
Caelo	Diltiazem hydrochloride	2504140I	1
Caelo	Diltiazem hydrochloride	251422/1	1
Caelo	Diltiazem hydrochloride	261115DHC	1
Caelo	Diltiazem hydrochloride	27101706	1
Caelo	Diltiazem hydrochloride	27101803	1
Caelo	Diltiazem hydrochloride	2760181	1
Caelo	Diltiazem hydrochloride	2818A-03562	1
Caelo	Diltiazem hydrochloride	3313U-03562	1
Caelo	Diltiazem hydrochloride	3442	1
Caelo	Diltiazem hydrochloride	514I-03562	1
Caelo	Diltiazem hydrochloride	6031302	1
Caelo	Diltiazem hydrochloride	7082005	1
Caelo	Diltiazem hydrochloride	8726	1
Caelo	Diltiazem hydrochloride	DIL/M-04511	1
Caelo	Diltiazem hydrochloride	DIL/M-19911	1
Caelo	Diltiazem hydrochloride	RT297	1
Caeol/Noweda	Diltiazem hydrochloride	17337018	1
Caeolo	Diltiazem hydrochloride	17337005	2
Caesar & Lorenz GmbH	Diltiazem hydrochloride	17043218	1
Caesar & Lorenz GmbH	Diltiazem hydrochloride	190841007	1
Caesar & Loretz / AHD	Diltiazem hydrochloride	19084107	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035018	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	190841007	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	19084107	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035002	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035014	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	20000622014	2
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035004	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	20000622007	2
Caesar & Loretz GmbH...	Diltiazem hydrochloride	19084106	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	19084105	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035010	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	190841007	2
Caesar & Loretz GmbH...	Diltiazem hydrochloride	1908410	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	190841007	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035002	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	190841004	5
Caesar & Loretz GmbH...	Diltiazem hydrochloride	190841005	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	19084110	1
Caesar & Loretz GmbH/AEP	Diltiazem hydrochloride	19084107	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/AHD	Diltiazem hydrochloride	21000035010	1
Caesar & Loretz GmbH/AHD	Diltiazem hydrochloride	21000035023	1
Caesar & Loretz GmbH/AHD	Diltiazem hydrochloride	22001215026	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	22001215008	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	22001215015	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	190841006	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035002	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035010	1
Caesar & Loretz GmbH/E	Diltiazem hydrochloride	20000622010	1
Caesar & Loretz GmbH/E	Diltiazem hydrochloride	21000035011	1
Caesar & Loretz GmbH/E	Diltiazem hydrochloride	22001215003	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	17337027	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035017	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035021	1
Caesar & Loretz GmbH/G	Diltiazem hydrochloride	21000035003	1
Caesar & Loretz GmbH/G	Diltiazem hydrochloride	21000035017	1
Caesar & Loretz GmbH/Gehe	Diltiazem hydrochloride	190841007	2
Caesar & Loretz GmbH/GEHE	Diltiazem hydrochloride	19084105	1
Caesar & Loretz GmbH/Gehe	Diltiazem hydrochloride	19084106	1
Caesar & Loretz GmbH/Gehe	Diltiazem hydrochloride	19084107	1
Caesar & Loretz GmbH/gehe	Diltiazem hydrochloride	19084108	1
Caesar & Loretz GmbH/Gehe	Diltiazem hydrochloride	20000622010	1
Caesar & Loretz GmbH/Gehe	Diltiazem hydrochloride	20000622014	1
Caesar & Loretz GmbH/Gehe	Diltiazem hydrochloride	21000035010	1
Caesar & Loretz GmbH/Gehe	Diltiazem hydrochloride	21000035011	1
Caesar & Loretz GmbH/Gehe	Diltiazem hydrochloride	21000035017	3
Caesar & Loretz GmbH/Gehe	Diltiazem hydrochloride	21000035021	1
Caesar & Loretz GmbH/gehe	Diltiazem hydrochloride	22001215008	1
Caesar & Loretz GmbH/Gehe	Diltiazem hydrochloride	22001215019	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	20000622008	2
Caesar & Loretz GmbH...	Diltiazem hydrochloride	20000622015	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035011	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	19084104	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	19084106	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035009	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035011	1
Caesar & Loretz GmbH/K	Diltiazem hydrochloride	21000035009	1
Caesar & Loretz GmbH/Kehr	Diltiazem hydrochloride	21000035023	1
Caesar & Loretz GmbH/Kehr	Diltiazem hydrochloride	22001215011	3
Caesar & Loretz GmbH...	Diltiazem hydrochloride	190841007	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	19084103	2
Caesar & Loretz GmbH...	Diltiazem hydrochloride	19084105	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	19084115	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035012	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	22001215007	7
Caesar & Loretz GmbH/Ph	Diltiazem hydrochloride	19084108	1
Caesar & Loretz GmbH/Ph	Diltiazem hydrochloride	20000622009	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	19084108	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	19268401	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	20000622003	2
Caesar & Loretz GmbH...	Diltiazem hydrochloride	20000622008	2
Caesar & Loretz GmbH...	Diltiazem hydrochloride	20000622015	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035003	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035004	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035008	6
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035017	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	190841	2
Caesar & Loretz GmbH...	Diltiazem hydrochloride	190841007	2
Caesar & Loretz GmbH...	Diltiazem hydrochloride	19084103	6
Caesar & Loretz GmbH...	Diltiazem hydrochloride	19084105	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Diltiazem hydrochloride	19084106	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	19084111	2
Caesar & Loretz GmbH...	Diltiazem hydrochloride	19084115	2
Caesar & Loretz GmbH...	Diltiazem hydrochloride	20000622009	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	20000622010	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035003	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035009	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035011	3
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035017	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	AP220802-01	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	17337027	1
Caesar & Loretz GmbH	Diltiazem hydrochloride	12133010	1
Caesar & Loretz GmbH	Diltiazem hydrochloride	17043218	1
Caesar & Loretz GmbH	Diltiazem hydrochloride	17043219	1
Caesar & Loretz GmbH	Diltiazem hydrochloride	17337009	1
Caesar & Loretz GmbH	Diltiazem hydrochloride	17337014	2
Caesar & Loretz GmbH	Diltiazem hydrochloride	17337018	1
Caesar & Loretz GmbH	Diltiazem hydrochloride	17337025	7
Caesar & Loretz GmbH	Diltiazem hydrochloride	17337026	1
Caesar & Loretz GmbH	Diltiazem hydrochloride	17337027	4
Caesar & Loretz GmbH	Diltiazem hydrochloride	18301109	3
Caesar & Loretz GmbH	Diltiazem hydrochloride	18301110	3
Caesar & Loretz GmbH	Diltiazem hydrochloride	18301111	8
Caesar & Loretz GmbH	Diltiazem hydrochloride	190841002	3
Caesar & Loretz GmbH	Diltiazem hydrochloride	190841005	5
Caesar & Loretz GmbH	Diltiazem hydrochloride	190841006	7
Caesar & Loretz GmbH	Diltiazem hydrochloride	190841007	9
Caesar & Loretz GmbH	Diltiazem hydrochloride	19084103	3
Caesar & Loretz GmbH	Diltiazem hydrochloride	19084104	2
Caesar & Loretz GmbH	Diltiazem hydrochloride	19084105	7
Caesar & Loretz GmbH	Diltiazem hydrochloride	19084106	9
Caesar & Loretz GmbH	Diltiazem hydrochloride	19084107	7
Caesar & Loretz GmbH	Diltiazem hydrochloride	19084108	10
Caesar & Loretz GmbH	Diltiazem hydrochloride	19084110	2
Caesar & Loretz GmbH	Diltiazem hydrochloride	19084111	1
Caesar & Loretz GmbH	Diltiazem hydrochloride	19084115	6
Caesar & Loretz GmbH	Diltiazem hydrochloride	19135410	4
Caesar & Loretz GmbH	Diltiazem hydrochloride	20000622003	4
Caesar & Loretz GmbH	Diltiazem hydrochloride	20000622007	1
Caesar & Loretz GmbH	Diltiazem hydrochloride	20000622008	1
Caesar & Loretz GmbH	Diltiazem hydrochloride	20000622009	8
Caesar & Loretz GmbH	Diltiazem hydrochloride	20000622010	10
Caesar & Loretz GmbH	Diltiazem hydrochloride	20000622011	10
Caesar & Loretz GmbH	Diltiazem hydrochloride	20000622015	5
Caesar & Loretz GmbH	Diltiazem hydrochloride	2000622003	1
Caesar & Loretz GmbH	Diltiazem hydrochloride	20C12-F03	1
Caesar & Loretz GmbH	Diltiazem hydrochloride	21000035001	9
Caesar & Loretz GmbH	Diltiazem hydrochloride	21000035002	9
Caesar & Loretz GmbH	Diltiazem hydrochloride	21000035003	12
Caesar & Loretz GmbH	Diltiazem hydrochloride	21000035004	2
Caesar & Loretz GmbH	Diltiazem hydrochloride	21000035008	6
Caesar & Loretz GmbH	Diltiazem hydrochloride	21000035009	7
Caesar & Loretz GmbH	Diltiazem hydrochloride	21000035010	9
Caesar & Loretz GmbH	Diltiazem hydrochloride	21000035011	8
Caesar & Loretz GmbH	Diltiazem hydrochloride	21000035012	5
Caesar & Loretz GmbH	Diltiazem hydrochloride	21000035013	4
Caesar & Loretz GmbH	Diltiazem hydrochloride	21000035016	5
Caesar & Loretz GmbH	Diltiazem hydrochloride	21000035017	10
Caesar & Loretz GmbH	Diltiazem hydrochloride	21000035021	6
Caesar & Loretz GmbH	Diltiazem hydrochloride	21000035023	8

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Diltiazem hydrochloride	220001215007	1
Caesar & Loretz GmbH	Diltiazem hydrochloride	22001215002	2
Caesar & Loretz GmbH	Diltiazem hydrochloride	22001215003	8
Caesar & Loretz GmbH	Diltiazem hydrochloride	22001215007	7
Caesar & Loretz GmbH	Diltiazem hydrochloride	22001215008	5
Caesar & Loretz GmbH	Diltiazem hydrochloride	22001215009	8
Caesar & Loretz GmbH	Diltiazem hydrochloride	22001215011	3
Caesar & Loretz GmbH	Diltiazem hydrochloride	22001215012	2
Caesar & Loretz GmbH	Diltiazem hydrochloride	22001215013	4
Caesar & Loretz GmbH	Diltiazem hydrochloride	22001215015	7
Caesar & Loretz GmbH	Diltiazem hydrochloride	22001215019	4
Caesar & Loretz GmbH	Diltiazem hydrochloride	22001215030	2
Caesar & Loretz GmbH	Diltiazem hydrochloride	B03-3662107	1
Caesar & Loretz GmbH	Diltiazem hydrochloride	F03-3719008	2
Caesar & Loretz GmbH...	Diltiazem hydrochloride	21000035021	1
Caesar & Loretz GmbH...	Diltiazem hydrochloride	22001215015	1
Caesar & Loretz/Geil...	Diltiazem hydrochloride	190841006	1
Caesar & Loretz/Geil...	Diltiazem hydrochloride	20000622011	1
Caesar & Loretz/Geil...	Diltiazem hydrochloride	21000035010	1
Caesar & Loretz/Noweda	Diltiazem hydrochloride	19084108	1
Caesar & Loretz/Noweda	Diltiazem hydrochloride	21000035003	1
Caesar & Loretz	Diltiazem hydrochloride	16190806	1
Caesar & Loretz	Diltiazem hydrochloride	17043202	1
Caesar & Loretz	Diltiazem hydrochloride	17043216	1
Caesar & Loretz	Diltiazem hydrochloride	17337012	1
CAESAR & LORETZ	Diltiazem hydrochloride	19084105	1
Caesar / Gehe	Diltiazem hydrochloride	16190806	1
Caesar&Loretz GmbH /Anzag	Diltiazem hydrochloride	15414302	1
Caesar&Loretz GmbH/Anzag	Diltiazem hydrochloride	14318412	1
Caesar&Loretz GmbH	Diltiazem hydrochloride	20000622010	1
Caesar&Loretz GmbH	Diltiazem hydrochloride	20000622011	1
Caesar&Loretz GmbH	Diltiazem hydrochloride	21000035003	1
Caesar&Loretz GmbH	Diltiazem hydrochloride	21000035016	1
Caeser und Loretz GmbH	Diltiazem hydrochloride	19084108	1
Caleo/ Noweda	Diltiazem hydrochloride	17337009	2
Caleo/ Noweda	Diltiazem hydrochloride	17337027	2
Caleo/gehe	Diltiazem hydrochloride	18301111	1
Caleo	Diltiazem hydrochloride	17043202	1
Cealo/Sanacorp	Diltiazem hydrochloride	14059514	1
Cealo/Sanacorp	Diltiazem hydrochloride	190841006	1
Cealo	Diltiazem hydrochloride	22001215008	1
Chiesi/Phoenix	Diltiazem hydrochloride	15230502	1
Divis Laboratories ...	Diltiazem hydrochloride	20J01-F11_374760	1
Divis's Laboratoris ...	Diltiazem hydrochloride	AZ-0560718	2
EuRho/Phönix	Diltiazem hydrochloride	14059514	1
Euro OTC	Diltiazem hydrochloride	16A18B07	1
Euro OTC	Diltiazem hydrochloride	17043216	1
Euro OTC	Diltiazem hydrochloride	17043228	1
Euro OTC	Diltiazem hydrochloride	17337005	1
Euro OTC	Diltiazem hydrochloride	17337027	1
Europharm / Gehe	Diltiazem hydrochloride	17H25-B01-343273	1
Fagon/Noweda	Diltiazem hydrochloride	18H09-B03-354798	1
Fagron	Diltiazem hydrochloride		2
Fagron	Diltiazem hydrochloride	10808-N01	1
Fagron	Diltiazem hydrochloride	10D28-N23	1
Fagron	Diltiazem hydrochloride	11-01-N08	1
Fagron	Diltiazem hydrochloride	11C14-N18	1
Fagron	Diltiazem hydrochloride	11E18-N04	3
Fagron	Diltiazem hydrochloride	11I01-N08	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Diltiazem hydrochloride	11J28-N05	1
Fagron	Diltiazem hydrochloride	12/12-N02	4
Fagron	Diltiazem hydrochloride	12/12-NO2	1
Fagron	Diltiazem hydrochloride	12d05-n07	1
Fagron	Diltiazem hydrochloride	12D05-N07	14
Fagron	Diltiazem hydrochloride	12D05-N070	1
Fagron	Diltiazem hydrochloride	12F19-N10	3
Fagron	Diltiazem hydrochloride	12F19-N100102/574	1
Fagron	Diltiazem hydrochloride	12I12-N02	2
Fagron	Diltiazem hydrochloride	12K07-N02	2
Fagron	Diltiazem hydrochloride	12l12-N02	1
Fagron	Diltiazem hydrochloride	13346902	1
Fagron	Diltiazem hydrochloride	13346915	1
Fagron	Diltiazem hydrochloride	135968-0009	2
Fagron	Diltiazem hydrochloride	13a02-n05	1
Fagron	Diltiazem hydrochloride	13A02N05	3
Fagron	Diltiazem hydrochloride	13A02-N05	9
Fagron	Diltiazem hydrochloride	13C14-B11-322642	1
Fagron	Diltiazem hydrochloride	13F13-N05	10
Fagron	Diltiazem hydrochloride	13G16_N05	1
Fagron	Diltiazem hydrochloride	13G16-N05	23
Fagron	Diltiazem hydrochloride	13J24-B04	3
Fagron	Diltiazem hydrochloride	13j24-b04-286569	1
Fagron	Diltiazem hydrochloride	13J24B04286569	3
Fagron	Diltiazem hydrochloride	13J24-B04-286569	11
Fagron	Diltiazem hydrochloride	13J24-B04-286570	1
Fagron	Diltiazem hydrochloride	13J24-B04-286571	2
Fagron	Diltiazem hydrochloride	14C12_B04_292757	1
Fagron	Diltiazem hydrochloride	14C12_B04-294133	1
Fagron	Diltiazem hydrochloride	14C12B04	1
Fagron	Diltiazem hydrochloride	14C12-B04	7
Fagron	Diltiazem hydrochloride	14C12-B04_294133	1
Fagron	Diltiazem hydrochloride	14C12-B04-292757	23
Fagron	Diltiazem hydrochloride	14c12-b04-292759	1
Fagron	Diltiazem hydrochloride	14C12-B04-292759	4
Fagron	Diltiazem hydrochloride	14C12-B04294133	1
Fagron	Diltiazem hydrochloride	14C12-B04-294133	6
Fagron	Diltiazem hydrochloride	14c12-b04-294134	1
Fagron	Diltiazem hydrochloride	14C12-B04-294134	1
Fagron	Diltiazem hydrochloride	14C12-B04-294135	2
Fagron	Diltiazem hydrochloride	14G22B08	1
Fagron	Diltiazem hydrochloride	14G22-B08	3
Fagron	Diltiazem hydrochloride	14g22-b08-299781	1
Fagron	Diltiazem hydrochloride	14G22-B08299781	2
Fagron	Diltiazem hydrochloride	14G22-B08-299781	13
Fagron	Diltiazem hydrochloride	14G22-B08-299782	6
Fagron	Diltiazem hydrochloride	14G22-B08-299783	1
Fagron	Diltiazem hydrochloride	15414313	1
Fagron	Diltiazem hydrochloride	15B12/B01305399	1
Fagron	Diltiazem hydrochloride	15B12-b01	1
Fagron	Diltiazem hydrochloride	15B12-B01	8
Fagron	Diltiazem hydrochloride	15B12-B01_305399	1
Fagron	Diltiazem hydrochloride	15B12-B01-305299	1
Fagron	Diltiazem hydrochloride	15b12-b01-305399	2
Fagron	Diltiazem hydrochloride	15B12B01305399	2
Fagron	Diltiazem hydrochloride	15B12-B01-305399	26
Fagron	Diltiazem hydrochloride	15b12-b01-305400	2
Fagron	Diltiazem hydrochloride	15B12B01305400	1
Fagron	Diltiazem hydrochloride	15B12-B01-305400	8
Fagron	Diltiazem hydrochloride	15B12-B01-305401	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Diltiazem hydrochloride	15G20-B02-310792	1
Fagron	Diltiazem hydrochloride	15G20-B08	3
Fagron	Diltiazem hydrochloride	15G20-B08-310792	1
Fagron	Diltiazem hydrochloride	15G20-B08-312065	13
Fagron	Diltiazem hydrochloride	15g20-b08-314375	1
Fagron	Diltiazem hydrochloride	15G20-B08-314375	7
Fagron	Diltiazem hydrochloride	16A14-B11-322153	1
Fagron	Diltiazem hydrochloride	16A18-B07	5
Fagron	Diltiazem hydrochloride	16A18B07316667	1
Fagron	Diltiazem hydrochloride	16A18-B07-316667	13
Fagron	Diltiazem hydrochloride	16A18B07316668	1
Fagron	Diltiazem hydrochloride	16a18-b07-318732	2
Fagron	Diltiazem hydrochloride	16A18-B07318732	1
Fagron	Diltiazem hydrochloride	16A18-B07-318732	16
Fagron	Diltiazem hydrochloride	16A18-B07-318733	3
Fagron	Diltiazem hydrochloride	16A18-B07-319570	3
Fagron	Diltiazem hydrochloride	16C14-B11	4
Fagron	Diltiazem hydrochloride	16c14-b11-211642	1
Fagron	Diltiazem hydrochloride	16C14B11320568	2
Fagron	Diltiazem hydrochloride	16C14-B11-320568	5
Fagron	Diltiazem hydrochloride	16c14-b11-320849	1
Fagron	Diltiazem hydrochloride	16C14B11320849	1
Fagron	Diltiazem hydrochloride	16C14-B11-320849	16
Fagron	Diltiazem hydrochloride	16c14-b11-322152	1
Fagron	Diltiazem hydrochloride	16C14B11322152	1
Fagron	Diltiazem hydrochloride	16C14-B11-322152	7
Fagron	Diltiazem hydrochloride	16C14-B11-322153	6
Fagron	Diltiazem hydrochloride	16C14-B11-322642	16
Fagron	Diltiazem hydrochloride	16G20-B03	4
Fagron	Diltiazem hydrochloride	16g20-b03-325903	1
Fagron	Diltiazem hydrochloride	16G20B03325903	1
Fagron	Diltiazem hydrochloride	16G20B03-325903	1
Fagron	Diltiazem hydrochloride	16G20-B03-325903	21
Fagron	Diltiazem hydrochloride	16G20-B03-328133	11
Fagron	Diltiazem hydrochloride	16G20-B03-328253	4
Fagron	Diltiazem hydrochloride	16GH20-B03-325903	1
Fagron	Diltiazem hydrochloride	16L19-B01	1
Fagron	Diltiazem hydrochloride	16L19-B01_330396	1
Fagron	Diltiazem hydrochloride	16l19-b01-330365	1
Fagron	Diltiazem hydrochloride	16L19-B01-330365	9
Fagron	Diltiazem hydrochloride	16L19-B01-330395	2
Fagron	Diltiazem hydrochloride	16L19B01330396	1
Fagron	Diltiazem hydrochloride	16L19-B01-330396	8
Fagron	Diltiazem hydrochloride	17043203	1
Fagron	Diltiazem hydrochloride	17043215	1
Fagron	Diltiazem hydrochloride	17337026	1
Fagron	Diltiazem hydrochloride	17D11-B11	6
Fagron	Diltiazem hydrochloride	17D11-B11-333704	16
Fagron	Diltiazem hydrochloride	17D-11-B11-333704	1
Fagron	Diltiazem hydrochloride	17D11-B11-333705	3
Fagron	Diltiazem hydrochloride	17D11-B11-334192	4
Fagron	Diltiazem hydrochloride	17d11b11334837	1
Fagron	Diltiazem hydrochloride	17D11-B11-334837	19
Fagron	Diltiazem hydrochloride	17d11-b11-336727	1
Fagron	Diltiazem hydrochloride	17D11B11336727	1
Fagron	Diltiazem hydrochloride	17D11-B11-336727	7
Fagron	Diltiazem hydrochloride	17H25-B01	5
Fagron	Diltiazem hydrochloride	17H25-B01-340697	18
Fagron	Diltiazem hydrochloride	17H25-B01-340698	5
Fagron	Diltiazem hydrochloride	17H25-B01-340699	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Diltiazem hydrochloride	17h25-b01-341596	1
Fagron	Diltiazem hydrochloride	17H25-B01341596	1
Fagron	Diltiazem hydrochloride	17H25-B01-341596	16
Fagron	Diltiazem hydrochloride	17H25-B01-341597	3
Fagron	Diltiazem hydrochloride	17H25B01-341598	1
Fagron	Diltiazem hydrochloride	17H25-B01-341598	2
Fagron	Diltiazem hydrochloride	17H25-B01-343272	1
Fagron	Diltiazem hydrochloride	17H25-B01-343273	11
Fagron	Diltiazem hydrochloride	17H25-Bo1-340697	1
Fagron	Diltiazem hydrochloride	18301110	2
Fagron	Diltiazem hydrochloride	18A29_B01_348861	1
Fagron	Diltiazem hydrochloride	18A29-01-347886	1
Fagron	Diltiazem hydrochloride	18A29-B01	16
Fagron	Diltiazem hydrochloride	18A-29-B01	1
Fagron	Diltiazem hydrochloride	18A29-B01-32907	1
Fagron	Diltiazem hydrochloride	18a29b01345623	1
Fagron	Diltiazem hydrochloride	18A29-B01-345623	17
Fagron	Diltiazem hydrochloride	18a29-b01-345624	1
Fagron	Diltiazem hydrochloride	18A29-B01-345624	1
Fagron	Diltiazem hydrochloride	18A29-B01-345625	2
Fagron	Diltiazem hydrochloride	18A29-B01-346694	12
Fagron	Diltiazem hydrochloride	18A29-B01-346695	4
Fagron	Diltiazem hydrochloride	18A29B01347886	2
Fagron	Diltiazem hydrochloride	18A29-B01-347886	22
Fagron	Diltiazem hydrochloride	18A29-B01-347887	5
Fagron	Diltiazem hydrochloride	18a29-b01-348861	1
Fagron	Diltiazem hydrochloride	18A29B01348861	2
Fagron	Diltiazem hydrochloride	18A29-B01-348861	29
Fagron	Diltiazem hydrochloride	18A29B01350964	1
Fagron	Diltiazem hydrochloride	18A29-B01-350964	5
Fagron	Diltiazem hydrochloride	18A29B01-352722	1
Fagron	Diltiazem hydrochloride	18A29-B01-352722	3
Fagron	Diltiazem hydrochloride	18A-29-B01-352722	1
Fagron	Diltiazem hydrochloride	18A29-B01-352723	6
Fagron	Diltiazem hydrochloride	18A29-B01-352907	18
Fagron	Diltiazem hydrochloride	18A29-B01-352909	4
Fagron	Diltiazem hydrochloride	18A29-B01-358861	1
Fagron	Diltiazem hydrochloride	18A29-Bo1-345623	1
Fagron	Diltiazem hydrochloride	18A-B01	1
Fagron	Diltiazem hydrochloride	18A-B01-352907	1
Fagron	Diltiazem hydrochloride	18H03-B03-358920	1
Fagron	Diltiazem hydrochloride	18H09_B03_354798	1
Fagron	Diltiazem hydrochloride	18H09_B03_358918	1
Fagron	Diltiazem hydrochloride	18H09_B03_362595	1
Fagron	Diltiazem hydrochloride	18H09-B03	32
Fagron	Diltiazem hydrochloride	18H09-B03_354798	1
Fagron	Diltiazem hydrochloride	18H09-B03_366219	1
Fagron	Diltiazem hydrochloride	18H09-B03-0008	1
Fagron	Diltiazem hydrochloride	18H09-B03-326596	1
Fagron	Diltiazem hydrochloride	18H09-B03-352908	2
Fagron	Diltiazem hydrochloride	18H09-B03-354798	20
Fagron	Diltiazem hydrochloride	18H09-B03-357183	8
Fagron	Diltiazem hydrochloride	18H09B03357184	2
Fagron	Diltiazem hydrochloride	18H09-B03-357184	5
Fagron	Diltiazem hydrochloride	18h09-b03-358917	1
Fagron	Diltiazem hydrochloride	18H09-b03-358917	1
Fagron	Diltiazem hydrochloride	18H09B03358917	1
Fagron	Diltiazem hydrochloride	18H09-B03-358917	33
Fagron	Diltiazem hydrochloride	18H-09-B03-358917	2
Fagron	Diltiazem hydrochloride	18h09b03358918	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Diltiazem hydrochloride	18H09B03358918	1
Fagron	Diltiazem hydrochloride	18H09-B03-358918	20
Fagron	Diltiazem hydrochloride	18H09B03358919	1
Fagron	Diltiazem hydrochloride	18H09B03-358919	1
Fagron	Diltiazem hydrochloride	18H09-B03-358919	9
Fagron	Diltiazem hydrochloride	18H09B03358920	2
Fagron	Diltiazem hydrochloride	18H09-B03-358920	5
Fagron	Diltiazem hydrochloride	18H09-B03-3589818	1
Fagron	Diltiazem hydrochloride	18H09-B03-3625905	1
Fagron	Diltiazem hydrochloride	18H09-B03-3625909	1
Fagron	Diltiazem hydrochloride	18h09-b03-362595	1
Fagron	Diltiazem hydrochloride	18H09-B03-362595	29
Fagron	Diltiazem hydrochloride	18H09B03-362596	1
Fagron	Diltiazem hydrochloride	18H09-B03-362596	22
Fagron	Diltiazem hydrochloride	18H09-B03-362596/AZ-0560718	1
Fagron	Diltiazem hydrochloride	18h09-b03-362599	2
Fagron	Diltiazem hydrochloride	18H09-B03362599	1
Fagron	Diltiazem hydrochloride	18H09-B03-362599	14
Fagron	Diltiazem hydrochloride	18H09-B03-362600	3
Fagron	Diltiazem hydrochloride	18H09B03366217	2
Fagron	Diltiazem hydrochloride	18H09-B03-366217	47
Fagron	Diltiazem hydrochloride	18-H09-B03-366217	1
Fagron	Diltiazem hydrochloride	18H09-B03366218	1
Fagron	Diltiazem hydrochloride	18H09-B03-366218	12
Fagron	Diltiazem hydrochloride	18-H09B03366218	1
Fagron	Diltiazem hydrochloride	18H09-B03-366219	8
Fagron	Diltiazem hydrochloride	18H09-B03-58918	1
Fagron	Diltiazem hydrochloride	18H09-B03-654798	1
Fagron	Diltiazem hydrochloride	18H09-B03-354798	1
Fagron	Diltiazem hydrochloride	18H09-B03-362596	1
Fagron	Diltiazem hydrochloride	18H09-B03-366218	1
Fagron	Diltiazem hydrochloride	18H19-B03-358918	2
Fagron	Diltiazem hydrochloride	18H-B03	1
Fagron	Diltiazem hydrochloride	18H09-B03-366219	1
Fagron	Diltiazem hydrochloride	190312702	1
Fagron	Diltiazem hydrochloride	190841308	1
Fagron	Diltiazem hydrochloride	19H09-B03-357184	1
Fagron	Diltiazem hydrochloride	20C12F03	1
Fagron	Diltiazem hydrochloride	20C12-F03	11
Fagron	Diltiazem hydrochloride	20C12-F03_371907	1
Fagron	Diltiazem hydrochloride	20C12-F03-3719007	1
Fagron	Diltiazem hydrochloride	20c12f03371907	1
Fagron	Diltiazem hydrochloride	20c12-f03-371907	1
Fagron	Diltiazem hydrochloride	20C12F03371907	1
Fagron	Diltiazem hydrochloride	20C12-F03-371907	38
Fagron	Diltiazem hydrochloride	20C12-F03-371908	4
Fagron	Diltiazem hydrochloride	20C12-F03-3733809	1
Fagron	Diltiazem hydrochloride	20C12F03373389	1
Fagron	Diltiazem hydrochloride	20C12-F03-373389	6
Fagron	Diltiazem hydrochloride	20c12-f03-374171	2
Fagron	Diltiazem hydrochloride	20c12-F03-374171	1
Fagron	Diltiazem hydrochloride	20C12F03374171	1
Fagron	Diltiazem hydrochloride	20C12-F03-374171	14
Fagron	Diltiazem hydrochloride	20C12-F03-371907	3
Fagron	Diltiazem hydrochloride	20J01-F11	5
Fagron	Diltiazem hydrochloride	20j01-f11-374760	3
Fagron	Diltiazem hydrochloride	20j01-F11-374760	1
Fagron	Diltiazem hydrochloride	20J01-F11-374760	29
Fagron	Diltiazem hydrochloride	20J01-F11-3747600	1
Fagron	Diltiazem hydrochloride	20J01F11374761	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Diltiazem hydrochloride	20J01-F11-374761	11
Fagron	Diltiazem hydrochloride	20J01-F11374763	1
Fagron	Diltiazem hydrochloride	20J01-F11-374763	7
Fagron	Diltiazem hydrochloride	20J01-F11-374764	12
Fagron	Diltiazem hydrochloride	20J01-F11-374765	1
Fagron	Diltiazem hydrochloride	212F11-803-216679	1
Fagron	Diltiazem hydrochloride	21D26-F02	3
Fagron	Diltiazem hydrochloride	21D26-F02-378333	32
Fagron	Diltiazem hydrochloride	21D26-F03-378339	3
Fagron	Diltiazem hydrochloride	21F11	1
Fagron	Diltiazem hydrochloride	21F11_b03_216679	1
Fagron	Diltiazem hydrochloride	21F11-803	1
Fagron	Diltiazem hydrochloride	21F11-803-216679	1
Fagron	Diltiazem hydrochloride	21F11-b03	1
Fagron	Diltiazem hydrochloride	21F11-B03	8
Fagron	Diltiazem hydrochloride	21F11-B03_221072	1
Fagron	Diltiazem hydrochloride	21F11-B03-213610	5
Fagron	Diltiazem hydrochloride	21F11-B03-213611	12
Fagron	Diltiazem hydrochloride	21F11-B03-216679	31
Fagron	Diltiazem hydrochloride	21F11B03216762	2
Fagron	Diltiazem hydrochloride	21F11-B03-216762	10
Fagron	Diltiazem hydrochloride	21F11-B03-218832	3
Fagron	Diltiazem hydrochloride	21F11-B03-218858	7
Fagron	Diltiazem hydrochloride	21F11-B03-218922	4
Fagron	Diltiazem hydrochloride	21F11-B03-2210071	1
Fagron	Diltiazem hydrochloride	21F11-B03-221071	22
Fagron	Diltiazem hydrochloride	21F11-B03-221072	1
Fagron	Diltiazem hydrochloride	21F11-B03-221073	1
Fagron	Diltiazem hydrochloride	21F11-B03-223064	7
Fagron	Diltiazem hydrochloride	21f11-bo3-216679	1
Fagron	Diltiazem hydrochloride	21F11-BO3-216679	1
Fagron	Diltiazem hydrochloride	21F11-BO3-216762	2
Fagron	Diltiazem hydrochloride	22/13-B07-223063	1
Fagron	Diltiazem hydrochloride	22082014A	1
Fagron	Diltiazem hydrochloride	22113-B07	1
Fagron	Diltiazem hydrochloride	22113-B07-223063	1
Fagron	Diltiazem hydrochloride	2213-B07-223063	1
Fagron	Diltiazem hydrochloride	221D-F02-378333	1
Fagron	Diltiazem hydrochloride	22I12-B07-223063	1
Fagron	Diltiazem hydrochloride	22I13-B07	1
Fagron	Diltiazem hydrochloride	22i13-B07-223063	1
Fagron	Diltiazem hydrochloride	22I13-B07-223063	13
Fagron	Diltiazem hydrochloride	22I13-B07-223065	5
Fagron	Diltiazem hydrochloride	22I13-B07-225364	1
Fagron	Diltiazem hydrochloride	22l13-B07	1
Fagron	Diltiazem hydrochloride	23C20-B02-227683	1
Fagron	Diltiazem hydrochloride	23C20-B02-228330	2
Fagron	Diltiazem hydrochloride	2798	1
Fagron	Diltiazem hydrochloride	3046333	1
Fagron	Diltiazem hydrochloride	362596	1
Fagron	Diltiazem hydrochloride	3713M-03562	1
Fagron	Diltiazem hydrochloride	371907	1
Fagron	Diltiazem hydrochloride	612213562	1
Fagron	Diltiazem hydrochloride	9J14-N17	1
Fagron	Diltiazem hydrochloride	AT-0810520	1
Fagron	Diltiazem hydrochloride	AZ-0100716	1
Fagron	Diltiazem hydrochloride	AZ-0150120	4
Fagron	Diltiazem hydrochloride	AZ-0350522	2
Fagron	Diltiazem hydrochloride	AZ-0440321	4
Fagron	Diltiazem hydrochloride	AZ-0440321/21F11-B03-221071	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Diltiazem hydrochloride	AZ-04600321	1
Fagron	Diltiazem hydrochloride	AZ-0460321	4
Fagron	Diltiazem hydrochloride	AZ-0470321	1
Fagron	Diltiazem hydrochloride	AZ0560718	1
Fagron	Diltiazem hydrochloride	AZ-0560718	18
Fagron	Diltiazem hydrochloride	AZ-0631216	10
Fagron	Diltiazem hydrochloride	AZ-0641216	4
Fagron	Diltiazem hydrochloride	az-0810520	1
Fagron	Diltiazem hydrochloride	AZ-0810520	9
Fagron	Diltiazem hydrochloride	AZ3500522	1
Fagron	Diltiazem hydrochloride	AZ-C150120	1
Fagron	Diltiazem hydrochloride	B03_2167602	1
Fagron	Diltiazem hydrochloride	B03-3625909	1
Fagron	Diltiazem hydrochloride	B03-3662107	4
Fagron	Diltiazem hydrochloride	B03-3662108	4
Fagron	Diltiazem hydrochloride	B07-2230603	1
Fagron	Diltiazem hydrochloride	Bo3-3626000	1
Fagron	Diltiazem hydrochloride	DIL/M-01314	1
Fagron	Diltiazem hydrochloride	DIL/M-0314	1
Fagron	Diltiazem hydrochloride	DIL/M-10515	2
Fagron	Diltiazem hydrochloride	DIL/M-13114	1
Fagron	Diltiazem hydrochloride	DIL/M-20215	1
Fagron	Diltiazem hydrochloride	DIL/M-21816	4
Fagron	Diltiazem hydrochloride	Dilt09122022	1
Fagron	Diltiazem hydrochloride	F01-3783303	1
Fagron	Diltiazem hydrochloride	F02-3783303	2
Fagron	Diltiazem hydrochloride	F03-3719007	9
Fagron	Diltiazem hydrochloride	F03-3719008	1
Fagron	Diltiazem hydrochloride	F03-3733809	1
Fagron	Diltiazem hydrochloride	F03-3741701	2
Fagron	Diltiazem hydrochloride	F03-374171	1
Fagron	Diltiazem hydrochloride	F11-3747600	5
Fagron	Diltiazem hydrochloride	F11-3747601	1
Fagron	Diltiazem hydrochloride	F11-3747603	1
Fagron	Diltiazem hydrochloride	F11-3747605	1
Fagron	Diltiazem hydrochloride	F11-374764	1
Fagron	Diltiazem hydrochloride	P-07041629/305400	1
Fagron	Diltiazem hydrochloride	P-09101821/348861	1
Fargon/AEP	Diltiazem hydrochloride	20C12-F03-371907	1
Fargon/AHD	Diltiazem hydrochloride	18A29-B01-352907	1
Fargon/Kehr	Diltiazem hydrochloride	16G20-B03-328133	1
Fargon/Krieger	Diltiazem hydrochloride	17H25-B1-340697	1
Fargon/Krieger	Diltiazem hydrochloride	18A29-B01-352907	1
Fargon/Krieger	Diltiazem hydrochloride	18H09-B03-354798	1
Fargon/Krieger	Diltiazem hydrochloride	18H09-B03-362595	1
Fargon/Noweda	Diltiazem hydrochloride	18H09-B03	1
Fargon/Phönix	Diltiazem hydrochloride	18H09-B03-358917	1
Fargon/Phönix	Diltiazem hydrochloride	20C12-F03-374171	1
Fargon/Phönix	Diltiazem hydrochloride	21F11-B03-216820	1
Fargon	Diltiazem hydrochloride	16C14-B11-320849	1
Fargon	Diltiazem hydrochloride	18A29-B01-348861	1
Fargon	Diltiazem hydrochloride	18A29-B01-352907	1
Fargon	Diltiazem hydrochloride	18H09-B03-362595	1
Fargon	Diltiazem hydrochloride	AZ-0810520	1
Fargon	Diltiazem hydrochloride	B03-3625905	1
Fargon	Diltiazem hydrochloride	F03-3719007	1
FGagron7Noweda	Diltiazem hydrochloride	B03-2136101	1
Fgron / Gehe	Diltiazem hydrochloride	17H25B01341596	1
Fiebig ek:12.27 01.08.12	Diltiazem hydrochloride	11/01-N08	1
Fiebig	Diltiazem hydrochloride	15230514	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fiebig	Diltiazem hydrochloride	16G20-B03-328133	1
Fiebig	Diltiazem hydrochloride	17043227	1
Fragon/ Gehe	Diltiazem hydrochloride	18h09b03366217	1
Fragon/Alliance	Diltiazem hydrochloride	21F11-Bo3-216679	1
Fragon/Noweda	Diltiazem hydrochloride	16L19-B01-330396	1
Fragon/Sanacorp	Diltiazem hydrochloride	18H09-B03-358918	1
Gatt-Koller	Diltiazem hydrochloride	22J02643	1
Gehe amax	Diltiazem hydrochloride	18H09-B03-354798	1
Gehe amax	Diltiazem hydrochloride	18H09-B03-366218	1
Gehe amax	Diltiazem hydrochloride	190841005	2
Gehe amax	Diltiazem hydrochloride	19084106	1
Gehe	Diltiazem hydrochloride	12133009	1
Gehe	Diltiazem hydrochloride	12133022	1
Gehe	Diltiazem hydrochloride	13346915	1
Gehe	Diltiazem hydrochloride	14C12-B04-292757	1
Gehe	Diltiazem hydrochloride	14G22-B08-299781	1
Gehe	Diltiazem hydrochloride	15230503	1
Gehe	Diltiazem hydrochloride	15414319	1
Gehe	Diltiazem hydrochloride	15B12-B01-305399	2
Gehe	Diltiazem hydrochloride	16190806	1
Gehe	Diltiazem hydrochloride	16190813	1
GEHE	Diltiazem hydrochloride	16190813	1
Gehe	Diltiazem hydrochloride	16L-19-B01-330365	1
Gehe	Diltiazem hydrochloride	17043202	1
GEHE	Diltiazem hydrochloride	17043217	1
Gehe	Diltiazem hydrochloride	17043218	1
Gehe	Diltiazem hydrochloride	17043219	1
Gehe	Diltiazem hydrochloride	17337005	1
GEHE	Diltiazem hydrochloride	17337025	2
Gehe	Diltiazem hydrochloride	17337026	1
Gehe	Diltiazem hydrochloride	17337027	1
Gehe	Diltiazem hydrochloride	17D11-B11	1
Gehe	Diltiazem hydrochloride	17d11-b11-334837	1
Gehe	Diltiazem hydrochloride	18301111	1
Gehe	Diltiazem hydrochloride	18A29-B01	1
Gehe	Diltiazem hydrochloride	18A29-B01-348861	1
Gehe	Diltiazem hydrochloride	18A29-B01-352907	1
Gehe	Diltiazem hydrochloride	18H09-B03	1
Gehe	Diltiazem hydrochloride	18H09-B03-358917	1
Gehe	Diltiazem hydrochloride	18H09-B03-358918	1
Gehe	Diltiazem hydrochloride	18H09-B03-362599	1
GEHE	Diltiazem hydrochloride	19084110	1
Gehe	Diltiazem hydrochloride	20000622009	1
Gehe	Diltiazem hydrochloride	20C12-F03	1
Gehe	Diltiazem hydrochloride	20C12-F03-371907	1
Gehe	Diltiazem hydrochloride	20J01-F11-374760	1
Gehe	Diltiazem hydrochloride	21000035002	1
Gehe	Diltiazem hydrochloride	21000035016	1
Gehe	Diltiazem hydrochloride	21D26-F02-378333	1
Gehe	Diltiazem hydrochloride	21F11-B03-213610	1
Gehe	Diltiazem hydrochloride	21F11-B03-221071	2
Gehe	Diltiazem hydrochloride	22001215009	1
Gehe	Diltiazem hydrochloride	22001215012	1
GEHE	Diltiazem hydrochloride	22001215018	1
Gehe	Diltiazem hydrochloride	22001215024	1
Gehe	Diltiazem hydrochloride	22I13-B07-223063	1
GEHE	Diltiazem hydrochloride	22I13-B07-223063	1
Gehe	Diltiazem hydrochloride	23C20-B02-228330	1
Gehe	Diltiazem hydrochloride	F11-3747600	1
Geilenkirchen	Diltiazem hydrochloride	17043218	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Geilenkirchen	Diltiazem hydrochloride	19084108	1
Hedinger GmbH	Diltiazem hydrochloride	16G20-B03	1
Jenne	Diltiazem hydrochloride	15414313	1
Jenne	Diltiazem hydrochloride	21000035017	1
Jenne	Diltiazem hydrochloride	22001215019	1
Jenne	Diltiazem hydrochloride	22001215030	1
Kehr	Diltiazem hydrochloride	17043228	1
Kehr	Diltiazem hydrochloride	22001215003	2
Kehr	Diltiazem hydrochloride	22001215030	2
Klenk	Diltiazem hydrochloride	18A29-B01-347886	1
Klosterring	Diltiazem hydrochloride	16190806	1
Krieger/Phönix	Diltiazem hydrochloride	AZ-0460321	1
Krieger	Diltiazem hydrochloride	22i13-B07-223063	1
Kuerzel	Diltiazem hydrochloride	13G16-N05	1
M/s.Piramal Enterpri...	Diltiazem hydrochloride	190841005	1
M/s.Piramal Enterpri...	Diltiazem hydrochloride	19084108	1
M/s/Noweda	Diltiazem hydrochloride	DIL/M-03519	4
Nachprüfung	Diltiazem hydrochloride		1
Noveda	Diltiazem hydrochloride	18A29-B01-348861	1
Noveda	Diltiazem hydrochloride	20000622011	1
Noweda 17.09.2019	Diltiazem hydrochloride	19084105	1
Noweda	Diltiazem hydrochloride	12133010	1
Noweda	Diltiazem hydrochloride	12133022	1
Noweda	Diltiazem hydrochloride	12133029	1
Noweda	Diltiazem hydrochloride	12176801	1
Noweda	Diltiazem hydrochloride	13346901	1
Noweda	Diltiazem hydrochloride	14318409	1
Noweda	Diltiazem hydrochloride	15230503	1
Noweda	Diltiazem hydrochloride	15414319	1
Noweda	Diltiazem hydrochloride	16190812	1
Noweda	Diltiazem hydrochloride	16L19-B01-330365	2
Noweda	Diltiazem hydrochloride	17334012	1
Noweda	Diltiazem hydrochloride	17337026	1
Noweda	Diltiazem hydrochloride	17D11-B11-334837	1
Noweda	Diltiazem hydrochloride	18H09B03358918	1
Noweda	Diltiazem hydrochloride	18H09-B03-362595	1
Noweda	Diltiazem hydrochloride	19084104	1
Noweda	Diltiazem hydrochloride	20000622011	1
Noweda	Diltiazem hydrochloride	20J01-F11-374760	1
Noweda	Diltiazem hydrochloride	21000035002	1
Noweda	Diltiazem hydrochloride	21000035003	1
Noweda	Diltiazem hydrochloride	21000035017	1
Noweda	Diltiazem hydrochloride	2100035010	1
Noweda	Diltiazem hydrochloride	21F11-B03	1
Noweda	Diltiazem hydrochloride	22001215007	2
Noweda	Diltiazem hydrochloride	22001215012	1
Noweda	Diltiazem hydrochloride	22001215018	1
Noweda	Diltiazem hydrochloride	22001215024	3
NOWEDA	Diltiazem hydrochloride	22001215030	1
Noweda	Diltiazem hydrochloride	2201215030	1
Noweda	Diltiazem hydrochloride	22113-B07-225364	1
Noweda	Diltiazem hydrochloride	22I13-B07-223063	1
Noweda	Diltiazem hydrochloride	22I13-B07-225364	1
Noweda	Diltiazem hydrochloride	22113-B07-225365	1
Noweda	Diltiazem hydrochloride	24000125007	1
p&m cosmetics/gehe	Diltiazem hydrochloride	17043217	1
Phoenix 14.03.2019 15,21EUR	Diltiazem hydrochloride	18A29-B01-345623	1
phoenix	Diltiazem hydrochloride	11/01-N08	1
Phoenix	Diltiazem hydrochloride	13346902	1
Phoenix	Diltiazem hydrochloride	13346914	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
phoenix	Diltiazem hydrochloride	14318412	1
Phoenix	Diltiazem hydrochloride	15230503	1
Phoenix	Diltiazem hydrochloride	17337005	1
Phoenix	Diltiazem hydrochloride	17337018	1
Phoenix	Diltiazem hydrochloride	18h09-b03	1
Phoenix	Diltiazem hydrochloride	18H09-B03-357183	1
Phoenix	Diltiazem hydrochloride	20000622014	1
Phoenix	Diltiazem hydrochloride	200101601	1
Phoenix	Diltiazem hydrochloride	20J01-F11	1
Phoenix	Diltiazem hydrochloride	20j01-f11-374763	1
Phoenix	Diltiazem hydrochloride	21000035001	2
Phoenix	Diltiazem hydrochloride	21000035003	1
Phoenix	Diltiazem hydrochloride	21000035013	3
Phoenix	Diltiazem hydrochloride	2100035004	1
Phoenix	Diltiazem hydrochloride	22001215024	1
Phoenix	Diltiazem hydrochloride	22001215030	1
Phoenix	Diltiazem hydrochloride	22I13-B07-223063	1
Phoenix	Diltiazem hydrochloride	22l13-B07-223063	1
Phoenix	Diltiazem hydrochloride	23G06-B07-234623	1
Phoenix	Diltiazem hydrochloride	AZ-0260423	1
Phoenix	Diltiazem hydrochloride	B03-3625906	1
Phönix Gotha	Diltiazem hydrochloride	15230503	1
Phönix, Caesar&Loret…	Diltiazem hydrochloride	19084115	1
Phönix/Fagon	Diltiazem hydrochloride	16A18-B07_318732	1
Phönix/Fargon	Diltiazem hydrochloride	18H09-B03-358917	1
Phönix/Fargon	Diltiazem hydrochloride	AZ-0560718	1
Phönix/Fargon	Diltiazem hydrochloride	F03-3719007	1
Phönix	Diltiazem hydrochloride	13196106	1
Phönix	Diltiazem hydrochloride	13F13-N05	1
phönix	Diltiazem hydrochloride	14059514	1
Phönix	Diltiazem hydrochloride	15212801	1
Phönix	Diltiazem hydrochloride	15414302	1
Phönix	Diltiazem hydrochloride	15G20-B08-310792	1
phönix	Diltiazem hydrochloride	16G20-B03-328133	1
PHÖNIX	Diltiazem hydrochloride	17043215	2
Phönix	Diltiazem hydrochloride	17043219	1
PHÖNIX	Diltiazem hydrochloride	17337004	2
Phönix	Diltiazem hydrochloride	17d11-b11-334837	1
Phönix	Diltiazem hydrochloride	18A29-B01-347886	1
Phönix	Diltiazem hydrochloride	18A29-B01-348861	1
Phönix	Diltiazem hydrochloride	18h09-b03-358917	1
Phönix	Diltiazem hydrochloride	18H09-B03358917	1
Phönix	Diltiazem hydrochloride	18H09-B03-362595	1
Phönix	Diltiazem hydrochloride	18H09-B03-366217	2
Phönix	Diltiazem hydrochloride	19084106	1
Phönix	Diltiazem hydrochloride	19084108	1
PHÖNIX	Diltiazem hydrochloride	19084108	1
Phönix	Diltiazem hydrochloride	20000622015	1
Phönix	Diltiazem hydrochloride	2000622003	1
Phönix	Diltiazem hydrochloride	20C12-F03-373389	1
Phönix	Diltiazem hydrochloride	21F11B03213611	1
phönix	Diltiazem hydrochloride	21F11-B03-221071	2
Phönix	Diltiazem hydrochloride	22001215024	3
Phönix	Diltiazem hydrochloride	22001215030	2
PHönix	Diltiazem hydrochloride	22001215030	1
Phönix	Diltiazem hydrochloride	2200121530	1
Phönix	Diltiazem hydrochloride	AZ-0350522	2
Phönix	Diltiazem hydrochloride	AZ-0560718	1
Phönix	Diltiazem hydrochloride	AZ-0951022	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Diltiazem hydrochloride	b03-3625906	1
Phönix	Diltiazem hydrochloride	f11-3747600	1
Piramal Healthcare L…	Diltiazem hydrochloride	12/12-N02	1
Piramal/Noweda	Diltiazem hydrochloride	DIL/M-02820	4
Piramaral Healthcare LTD.	Diltiazem hydrochloride	12F19-N10	1
Röntgen	Diltiazem hydrochloride	18A29-B01-350964	1
Sanacop	Diltiazem hydrochloride	14059523	1
Sanacorp /Fargron	Diltiazem hydrochloride	16G20-B03-325903	1
Sanacorp WE 17.02.17…	Diltiazem hydrochloride	16190806	1
Sanacorp, 18.02.17, …	Diltiazem hydrochloride	16190807	1
Sanacorp	Diltiazem hydrochloride	11134115	4
Sanacorp	Diltiazem hydrochloride	11134121	2
Sanacorp	Diltiazem hydrochloride	11J28-04511	1
Sanacorp	Diltiazem hydrochloride	12/12-N02	2
Sanacorp	Diltiazem hydrochloride	12133010	1
Sanacorp	Diltiazem hydrochloride	12I12-N02	1
Sanacorp	Diltiazem hydrochloride	13j24-b04-286569	1
Sanacorp	Diltiazem hydrochloride	14c12-b04-292757	1
Sanacorp	Diltiazem hydrochloride	17043217	1
Sanacorp	Diltiazem hydrochloride	17337005	1
Sanacorp	Diltiazem hydrochloride	17337009	1
Sanacorp	Diltiazem hydrochloride	17337026	2
Sanacorp	Diltiazem hydrochloride	18301111	2
Sanacorp	Diltiazem hydrochloride	18H09-B03	2
Sanacorp	Diltiazem hydrochloride	190841006	1
Sanacorp	Diltiazem hydrochloride	19084104	1
Sanacorp	Diltiazem hydrochloride	19084106	1
Sanacorp	Diltiazem hydrochloride	19084107	1
Sanacorp	Diltiazem hydrochloride	21000035003	1
Sanacorp	Diltiazem hydrochloride	21000035009	1
Sanacorp	Diltiazem hydrochloride	22001215007	2
Sanacorp	Diltiazem hydrochloride	22001215009	1
Sanacorp	Diltiazem hydrochloride	22001215012	1
Sanacorp	Diltiazem hydrochloride	22001215029	1
Sanacorp	Diltiazem hydrochloride	22I13-B07-223063	1
sanacorp	Diltiazem hydrochloride	23001896006	1
Sanacorp	Diltiazem hydrochloride	23G06-B07-234623	1
Sanacorp	Diltiazem hydrochloride	3216679	1
Sanacorp	Diltiazem hydrochloride	Fargon	1
sittig	Diltiazem hydrochloride	14G22-B08-299781	1
VDL;18.02.15;15,95EUR	Diltiazem hydrochloride	14059514	1
Wepa / Wepa	Diltiazem hydrochloride	17043218	1

- 231 512 spectra from 1515 *Apo-Ident* customers from a total of 48 565 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Diltiazem hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Diltiazem hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	300	0	201 784
Type C	0	4376	179	231 512

The substance/substance group *Diltiazem hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.0000 %)
Type C	100.0000 % (> 99.9007 %)	96.0703 % (> 96.0044 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21270	22631	27.41	88.30
21300	22631	12.72	88.77
21406	22631	11.96	88.74
21407	22631	12.46	96.73
22631	22631	0.00	100.37
23015	23325	22.54	94.39
23016	22631	26.58	96.56
23325	23325	0.00	95.90
25365	22631	17.27	102.15

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Diphenhydramine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20186-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Diphenhydramine hydrochloride; Diphenhydramini hydrochloridum

Special notes

When selecting the *Diphenhydramine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Diphenhydramine hydrochloride	7	5	65

Second-stage model

For differentiation of the substance/substance group *Diphenhydramine hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Diphenhydramine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Doxepin hydrochloride	79.41	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Diphenhydramine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Diphenhydramine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Diphenhydramine hydrochloride	12329816	21304	40	20121119
Caelo	Diphenhydramine hydrochloride	12329816	21464	60	20121119
Caelo	Diphenhydramine hydrochloride	16004901	23235	40	20160122
Caelo	Diphenhydramine hydrochloride	180082	24755	40	20180126*
Caelo	Diphenhydramine hydrochloride	22002760	26361	30	20220923*
Caelo	Diphenhydramine hydrochloride	22002760	26361SI	20	20220923*
Fagron	Diphenhydramine hydrochloride	16C25-B03-331026	23262	40	AR-17-FG-015432-02
Fagron	Diphenhydramine hydrochloride	18K28-B02-358954	24702	40	20181219
Fagron	Diphenhydramine hydrochloride	20G03-F08-374141	25746	50	20200928

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Diphenhydramine - hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 602 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Diphenhydramine - hydrochloride*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Diphenhydramine hydrochloride	15072617	23206	40
Caelo	Diphenhydramine hydrochloride	172276	23803	40
Caelo	Diphenhydramine hydrochloride	183010	24390	40
Caelo	Diphenhydramine hydrochloride	22003785	26717	40
Caelo	Diphenhydramine hydrochloride	23001022	26836	40
Caelo	Diphenhydramine hydrochloride	22003785	26717SI	20
Caelo	Diphenhydramine hydrochloride	23001022	26836SI	20

- 201 844 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 206 spectra from 104 *Apo-Ident* customers from 67 batches from the substance/substance group *Diphenhydramine hydrochloride*.

- Among them are spectra of independent samples from 65 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Diphenhydramine hydrochloride	21000109013	1
	Diphenhydramine hydrochloride	22002760004	2
	Diphenhydramine hydrochloride	22002760007	1
	Diphenhydramine hydrochloride	22003785002	1
Caelo	Diphenhydramine hydrochloride		1
Caelo	Diphenhydramine hydrochloride	10122030	1
Caelo	Diphenhydramine hydrochloride	12007702	1
Caelo	Diphenhydramine hydrochloride	12007713	2
Caelo	Diphenhydramine hydrochloride	12007715	2
Caelo	Diphenhydramine hydrochloride	12007716	1
Caelo	Diphenhydramine hydrochloride	12007721	2
Caelo	Diphenhydramine hydrochloride	12329805	1
Caelo	Diphenhydramine hydrochloride	12329815	2
Caelo	Diphenhydramine hydrochloride	13100462	1
Caelo	Diphenhydramine hydrochloride	13331810	2
Caelo	Diphenhydramine hydrochloride	13331813	1
Caelo	Diphenhydramine hydrochloride	13343104	1
Caelo	Diphenhydramine hydrochloride	15072602	4
Caelo	Diphenhydramine hydrochloride	15072603	5
Caelo	Diphenhydramine hydrochloride	15072608	1
Caelo	Diphenhydramine hydrochloride	15072609	6
Caelo	Diphenhydramine hydrochloride	15072614	12
Caelo	Diphenhydramine hydrochloride	15072617	3
Caelo	Diphenhydramine hydrochloride	15072630	1
Caelo	Diphenhydramine hydrochloride	15220402	1
Caelo	Diphenhydramine hydrochloride	15220403	8
Caelo	Diphenhydramine hydrochloride	15220404	3
Caelo	Diphenhydramine hydrochloride	15220405	3
Caelo	Diphenhydramine hydrochloride	16004905	1
Caelo	Diphenhydramine hydrochloride	16004908	3
Caelo	Diphenhydramine hydrochloride	16004910	8
Caelo	Diphenhydramine hydrochloride	18008201	5
Caelo	Diphenhydramine hydrochloride	18008202	3
Caelo	Diphenhydramine hydrochloride	18008205	5
Caelo	Diphenhydramine hydrochloride	18008208	10
Caelo	Diphenhydramine hydrochloride	18108407	1
Caelo	Diphenhydramine hydrochloride	1814A-01339	1
Caelo	Diphenhydramine hydrochloride	18168403	3
Caelo	Diphenhydramine hydrochloride	18168407	17
Caelo	Diphenhydramine hydrochloride	1912I-01339	1
Caelo	Diphenhydramine hydrochloride	2000239001	1
Caelo	Diphenhydramine hydrochloride	20002393001	4
Caelo	Diphenhydramine hydrochloride	20071502	1
Caelo	Diphenhydramine hydrochloride	2041403	1
Caelo	Diphenhydramine hydrochloride	21000108002	1
Caelo	Diphenhydramine hydrochloride	21000109007	2
Caelo	Diphenhydramine hydrochloride	21000109013	1
Caelo	Diphenhydramine hydrochloride	22003785002	1
Caelo	Diphenhydramine hydrochloride	2215I-01339	1
Caelo	Diphenhydramine hydrochloride	25071306	1
Caelo	Diphenhydramine hydrochloride	2517M-01339	1
Caelo	Diphenhydramine hydrochloride	2818A-01339	1
Caelo	Diphenhydramine hydrochloride	3071715	1
Caelo	Diphenhydramine hydrochloride	31031508	1
Caelo	Diphenhydramine hydrochloride	5121204	1
Caelo	Diphenhydramine hydrochloride	8072001	1
Caeolo	Diphenhydramine hydrochloride	18008205	1
Caesar & Loretz GmbH...	Diphenhydramine hydrochloride	18168407	2
Caesar & Loretz GmbH...	Diphenhydramine hydrochloride	18168407	1
Caesar & Loretz GmbH...	Diphenhydramine hydrochloride	21000108002	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH…	Diphenhydramine hydrochloride	21000109007	2
Caesar & Loretz GmbH	Diphenhydramine hydrochloride	18008208	1
Caesar & Loretz GmbH	Diphenhydramine hydrochloride	18168407	13
Caesar & Loretz GmbH	Diphenhydramine hydrochloride	20002393004	1
Caesar & Loretz GmbH	Diphenhydramine hydrochloride	21000108003	1
Caesar & Loretz GmbH	Diphenhydramine hydrochloride	21000109003	1
Caesar & Loretz GmbH	Diphenhydramine hydrochloride	21000109007	4
Caesar & Loretz Hilden	Diphenhydramine hydrochloride	16004905	1
Caesar & Loretz Hilden	Diphenhydramine hydrochloride	18008205	1
Caesar & Loretz Hilden	Diphenhydramine hydrochloride	18168403	1
Caesar & Loretz Hilden	Diphenhydramine hydrochloride	18168407	2
Caesar & Loretz Hilden	Diphenhydramine hydrochloride	20002393001	2
Caesar/Noweda	Diphenhydramine hydrochloride	12007714	1
Fagron	Diphenhydramine hydrochloride	12F28-N01	1
Fagron	Diphenhydramine hydrochloride	12J04-N02	1
Fagron	Diphenhydramine hydrochloride	13A14-B40-293346	1
Fagron	Diphenhydramine hydrochloride	15072614	1
Fagron	Diphenhydramine hydrochloride	16C25-B03-331026	1
Finze	Diphenhydramine hydrochloride	9F05-N04	2
Gatt-Koller	Diphenhydramine hydrochloride	21J02410	1
Gatt-Koller	Diphenhydramine hydrochloride	606030315	1
Gehe	Diphenhydramine hydrochloride	12329815	1
Jenne	Diphenhydramine hydrochloride	18008208	1
L30	Diphenhydramine hydrochloride	18008201	1
Noweda	Diphenhydramine hydrochloride	12007716	1
Noweda	Diphenhydramine hydrochloride	15220402	1
PHOENIX 29.01.2013	Diphenhydramine hydrochloride	120208	1
Phönix WE: 07.01.14 …	Diphenhydramine hydrochloride	12329805	1
Recordati/Noweda	Diphenhydramine hydrochloride	17100490	1
Sanacorp	Diphenhydramine hydrochloride	12329805	1
Sanacorp	Diphenhydramine hydrochloride	15072608	1
Sanacorp	Diphenhydramine hydrochloride	15072617	1
Sanacorp	Diphenhydramine hydrochloride	16004908	1
Supriya/Noweda	Diphenhydramine hydrochloride	20002393004	1

- 235 861 spectra from 1515 *Apo-Ident* customers from a total of 49 192 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Diphenhydramine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Diphenhydramine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	240	0	201 844
Type C	0	193	13	235 861

The substance/substance group *Diphenhydramine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	93.6893 % (> 92.2330 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21304	23262	18.78	102.26
21464	23262	16.09	102.07
23235	23262	17.99	101.77
23262	23262	0.00	109.33
24702	23262	9.02	107.35
24755	24755	0.00	101.41
25746	23262	10.05	102.35
26361	26361	0.00	102.31

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Diphenylcyclopropenone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10003690-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Diphenylcyclopropenone; Diphenylcyclopropenonum

Special notes

When selecting the *Diphenylcyclopropenone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Diphenylcyclopropenone	7	3	12

Second-stage model

For differentiation of the substance/substance group *Diphenylcyclopropenone* the following second-stage model is used:

- Submodel 18

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Diphenylcyclopropenone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium benzoate	45.05	27.24
Dithranol	113.76	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Diphenylcyclopropenone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Diphenylcyclopropenone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Diphenylcyclopropenone	12L17-N07	20934	40	1407599
Fagron	Diphenylcyclopropenone	13I26-N12	21342	40	1504598
Fagron	Diphenylcyclopropenone	13I26-N12	21539	35	20130920
Fagron	Diphenylcyclopropenone	16F02-B10-329708	23070	40	1902476
Fagron	Diphenylcyclopropenone	16F02-B10-326265	23071	40	20160822
Fagron	Diphenylcyclopropenone	20I09-F02-374243	25585	40	20201016
Fagron	Diphenylcyclopropenone	20J27-F06-374823	25741	50	20201109
Fagron	Diphenylcyclopropenone	22D27-B01-226151	26540	40	20220630
Fagron	Diphenylcyclopropenone	22D27-B01-226151	26540SI	20	20220630

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 345 spectra of 9 reference samples from the substance/substance group *Diphenylcyclopropenone*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 617 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 3 reference samples from the substance/substance group *Diphenylcyclopropenone*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Diphenylcyclopropenone	15J12-B01-316620	22362	60
Fagron	Diphenylcyclopropenone	18I03-B04-356833	24582	40
Fagron	Diphenylcyclopropenone	19K26-F01-367396	25189	40

- 201 944 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 16 spectra from 13 *Apo-Ident* customers from 13 batches from the substance/substance group *Diphenylcyclopropenone*.
- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Diphenylcyclopropenone	17B-13B02-334769	1
Fagron	Diphenylcyclopropenone	1(17B13-B02-34977)	1
Fagron	Diphenylcyclopropenone	16F02B10324263	1
Fagron	Diphenylcyclopropenone	16F02-B10-327812	3
Fagron	Diphenylcyclopropenone	18I03B04	1
Fagron	Diphenylcyclopropenone	18I-03-B04	1
Fagron	Diphenylcyclopropenone	18I03-B04_356833	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Diphenylcyclopropenone	19K26-F01-367396	1
Fagron	Diphenylcyclopropenone	20J27-F06-374823	1
Fagron	Diphenylcyclopropenone	35-16-I-95P3117	1
Fagron	Diphenylcyclopropenone	35-17-II-57P3503	1
Fiebig	Diphenylcyclopropenone	17B13-B02-334769	1
Frago/Noweda	Diphenylcyclopropenone	16F02-B10-324263	2

- 236 051 spectra from 1515 *Apo-Ident* customers from a total of 49 245 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Diphenylcyclopropenone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Diphenylcyclopropenone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	345	0	152 617
Type B	0	140	0	201 944
Type C	0	16	0	236 051

The substance/substance group *Diphenylcyclopropenone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2609 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20934	20934	0.00	102.33
21342	21342	0.00	274.97
21539	21342	4.51	283.16
23070	23070	0.00	93.22
23071	21342	64.38	277.20
25585	20934	35.56	113.62
25741	20934	12.55	107.77
26540	20934	39.01	96.11

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Dithranol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20032-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Dithranol; Dithranolum

Special notes

When selecting the *Dithranol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Dithranol	11	5	154

Second-stage model

For differentiation of the substance/substance group *Dithranol* the following second-stage model is used:

- Submodel 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Dithranol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	114.21	–
⋮	⋮	⋮
Sodium salicylate	>50	34.64
Dequalinium chloride	>50	36.10
Acetylsalicylic acid	>50	51.98
Benzoic acid	>50	59.17
Eosin Y	>50	161.16
Oxytetracycline hydrochloride	>50	269.52
Levothyroxin sodium	>50	567.21
Tannin	>50	1207.10

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Dithranol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Dithranol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Dithranol	18115302	24169	40	1811302
Caelo	Dithranol	18190604	24429	40	1904372
Caelo	Dithranol	190868	24501	40	20190426*
Caelo	Dithranol	190550	24503	40	20190426*
Caelo	Dithranol	20002967002	25429	30	2102141
Caelo	Dithranol	20002967	25646	40	20201021*
Euro OTC	Dithranol	1702022-01	24153	40	1809448
Euro OTC	Dithranol	2201006	25960	40	20220209*
Fagron	Dithranol	18B23-B05-348137	24172	40	20180430
Fagron	Dithranol	20K20-B04-203566	25502	40	20201127
Fagron	Dithranol	22F11-B02-223754	26452	40	230502386

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 430 spectra of 11 reference samples from the substance/substance group *Dithranol*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 532 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 250 spectra of 8 reference samples from the substance/substance group *Dithranol*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Audor Pharma	Dithranol	APOP_DNL/11/17/001D	24173	40
Caelo	Dithranol	24000565	27320	40
Euro OTC	Dithranol	2001025	25101	40
Euro OTC	Dithranol	2004028	25472	40
Euro OTC	Dithranol	2409010	27455	40
Caelo	Dithranol	24000565	27320SI	20
Euro OTC	Dithranol	2201006	25960SI†	10
Euro OTC	Dithranol	2409010	27455SI	20

- 201 834 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 566 spectra from 385 *Apo-Ident* customers from 169 batches from the substance/substance group *Dithranol*.
- Among them are spectra of independent samples from 153 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Dithranol	21000824004301221/4	1
	Dithranol	21I17-B01-213565	1
	Dithranol	22001422005	11
	Dithranol	22001422012	1
	Dithranol	2200142205	1
	Dithranol	2201006-01	1
	Dithranol	2201006-04	5
	Dithranol	2201006-05	2
	Dithranol	22F11-B02-219586	1
	Dithranol	22F11-B02-226170	5
	Dithranol	23F15-B01-231257	1
	Dithranol	23F15-BO1-231257	1
	Dithranol	23H22-B11-237978	1
	Dithranol	24000565004	2
	Dithranol	24F28-B29-002279	1
	Dithranol	B29-0022708	1
	Dithranol	OP-DNL-C1-001/22	1
11,41	Dithranol	23F15-B01-231257	1
AHC	Dithranol	2201006-01	1
AHD	Dithranol	1702022-04	1
AHD	Dithranol	21000824001	1
AHD	Dithranol	22001422005	1
AHD	Dithranol	APDT/386/2012D	1
Alliance	Dithranol	22001006-05	1
Alliance	Dithranol	22001422005	1
Alliance	Dithranol	2201006-05	1
Anzag	Dithranol		2
Anzag	Dithranol	120302502	1
Audor Pharma	Dithranol		15
Audor Pharma	Dithranol	11/11/002D	1
Audor Pharma	Dithranol	28(APOP-DNL/11/17/0	1
Audor Pharma	Dithranol	AOOP-DNL/11/17002S	1
Audor Pharma	Dithranol	APDT/351/2010D	1
Audor Pharma	Dithranol	APDT/365/2011	2
Audor Pharma	Dithranol	APDT/365/2011D	1
Audor Pharma	Dithranol	APDT/375/2012D	8
Audor Pharma	Dithranol	APDT/450/2016D	1
Audor Pharma	Dithranol	APDT/471/2017D	5
Audor Pharma	Dithranol	APDT3752012D	1
Audor Pharma	Dithranol	APDT3902013D	1
Audor Pharma	Dithranol	APO-DNL/11/17/001-1D	1
Audor Pharma	Dithranol	APOP-DNL/11/17/0002	1
Audor Pharma	Dithranol	ApOPDNL/11/17/001	1
Audor Pharma	Dithranol	APOP-DNL/11/17/001	2
Audor Pharma	Dithranol	APOP-DNL/11/17/001-1	3
Audor Pharma	Dithranol	APOPDNL/11/17/001-1D	1
Audor Pharma	Dithranol	APOP-DNL/11/17/001D	4

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Audor Pharma	Dithranol	APOP-DNL/11/17/001-D	4
Audor Pharma	Dithranol	APOP-DNL/11/17/002	4
Audor Pharma	Dithranol	apop-dnl/11/17/002d	1
Audor Pharma	Dithranol	APOP-DNL/11/17/002D	2
Audor Pharma	Dithranol	APOP-DNL/11/17001-1	1
Audor Pharma	Dithranol	APOP-DNL/11/17001-1D	1
Audor Pharma	Dithranol	APOP-DNL11170011D	1
Audor Pharma	Dithranol	APOPDNL1117002D	1
Audor Pharma	Dithranol	APQP-DNL/11/17/002D	1
Audor Pharma	Dithranol	DT/351/2010D	1
Audor Pharma	Dithranol	DT/375/2012D	2
Audor Pharma	Dithranol	OP-DNL/11/17/0001	1
Audor Pharma	Dithranol	OP-DNL/11/17/001	1
Audor Pharma	Dithranol	OP-DNL/11/17/001-1D	1
Caelo	Dithranol		2
Caelo	Dithranol	11064501	1
Caelo	Dithranol	12014502	1
Caelo	Dithranol	12014504	2
Caelo	Dithranol	1203025-02	1
Caelo	Dithranol	1212I-01274	1
Caelo	Dithranol	12236809	1
Caelo	Dithranol	12236811	4
Caelo	Dithranol	12375302	4
Caelo	Dithranol	12375305	1
Caelo	Dithranol	12375403	1
Caelo	Dithranol	12375601	1
Caelo	Dithranol	13120502	1
Caelo	Dithranol	13120503	1
Caelo	Dithranol	13120504	1
Caelo	Dithranol	13120702	1
Caelo	Dithranol	14101715	1
Caelo	Dithranol	1702022-01	1
Caelo	Dithranol	1702022-04	1
Caelo	Dithranol	18055001	1
Caelo	Dithranol	18115302	3
Caelo	Dithranol	18115306	3
Caelo	Dithranol	18115308	3
Caelo	Dithranol	18B23-B05-348137	1
Caelo	Dithranol	19055001	7
Caelo	Dithranol	19086804	3
Caelo	Dithranol	19204604	3
Caelo	Dithranol	19204605	5
Caelo	Dithranol	192939004	11
Caelo	Dithranol	192939005	3
Caelo	Dithranol	200000243003	1
Caelo	Dithranol	20000243003	13
Caelo	Dithranol	200004097004	1
Caelo	Dithranol	20001097004	1
Caelo	Dithranol	20002967002	1
Caelo	Dithranol	20004097001	6
Caelo	Dithranol	20004097002	1
Caelo	Dithranol	20004097004	8
Caelo	Dithranol	210000824001	1
Caelo	Dithranol	210008240007	1
Caelo	Dithranol	21000824001	20
Caelo	Dithranol	21000824002	2
Caelo	Dithranol	21000824004	25
Caelo	Dithranol	21000824007	14
Caelo	Dithranol	2100824004	1
Caelo	Dithranol	27111206	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dithranol	7/2020	1
Caelo	Dithranol	APDT/3652011D	1
Caelo	Dithranol	APDT/375/2012D	3
Caelo	Dithranol	APOP-DNL/11/17/001-1	1
Caelo	Dithranol	B04-2035606	1
Caesar & Loretz GmbH...	Dithranol	192939004	1
Caesar & Loretz GmbH...	Dithranol	21000824004	1
Caesar & Loretz GmbH...	Dithranol	192939004	1
Caesar & Loretz GmbH...	Dithranol	20000243002	1
Caesar & Loretz GmbH...	Dithranol	21000824004	1
Caesar & Loretz GmbH/Gehe	Dithranol	21000824001	1
Caesar & Loretz GmbH/Gehe	Dithranol	21000824004	1
Caesar & Loretz GmbH/Gehe	Dithranol	21000824007	1
Caesar & Loretz GmbH...	Dithranol	21000824007	2
Caesar & Loretz GmbH...	Dithranol	20004097001	1
Caesar & Loretz GmbH...	Dithranol	21000824002	1
Caesar & Loretz GmbH...	Dithranol	20000243004	1
Caesar & Loretz GmbH...	Dithranol	20004097001	1
Caesar & Loretz GmbH...	Dithranol	21000824007	2
Caesar & Loretz GmbH	Dithranol	1702022-04	1
Caesar & Loretz GmbH	Dithranol	19055001	2
Caesar & Loretz GmbH	Dithranol	19086804	1
CAESAR & LORETZ GMBH	Dithranol	192939004	1
Caesar & Loretz GmbH	Dithranol	192939005	1
Caesar & Loretz GmbH	Dithranol	20000243003	3
Caesar & Loretz GmbH	Dithranol	20000243004	1
Caesar & Loretz GmbH	Dithranol	20002967002	1
Caesar & Loretz GmbH	Dithranol	20004097001	7
Caesar & Loretz GmbH	Dithranol	20004097002	2
Caesar & Loretz GmbH	Dithranol	20004097004	5
Caesar & Loretz GmbH	Dithranol	21000824001	5
Caesar & Loretz GmbH	Dithranol	21000824003	1
Caesar & Loretz GmbH	Dithranol	21000824004	5
Caesar & Loretz GmbH	Dithranol	21000824007	3
Caesar & Loretz GmbH	Dithranol	22001422002	1
Caesar & Loretz GmbH	Dithranol	22001422005	1
Cealo	Dithranol	20004097004	2
Ceasar & Loretz GmbH...	Dithranol	19204605	1
EuRho / Noweda	Dithranol	2004028-01	1
EuRho/ Sanacorp	Dithranol	2201006-01	1
EuRho/Phoenix	Dithranol	2001025-01	2
EuRho/Sanacorp	Dithranol	2004028	1
EuRho	Dithranol	1203025-01	1
EuRho	Dithranol	2201006-03	1
Euro OTC	Dithranol		1
Euro OTC	Dithranol	1008011-01	1
Euro OTC	Dithranol	1008011-02	2
Euro OTC	Dithranol	1203025-01	2
Euro OTC	Dithranol	1203025-02	14
Euro OTC	Dithranol	1311029-01	1
Euro OTC	Dithranol	1702002-04	1
Euro OTC	Dithranol	17020022-02	1
Euro OTC	Dithranol	170202-01	1
Euro OTC	Dithranol	1702021	1
Euro OTC	Dithranol	1702021-02	2
Euro OTC	Dithranol	170202103	1
Euro OTC	Dithranol	1702021-03	13
Euro OTC	Dithranol	1702021-0301/2021	1
Euro OTC	Dithranol	1702022-01	2
Euro OTC	Dithranol	1702022-02	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Dithranol	1702022-04	12
Euro OTC	Dithranol	20004097002	1
Euro OTC	Dithranol	200102501	2
Euro OTC	Dithranol	2001025-01	26
Euro OTC	Dithranol	200402801	1
Euro OTC	Dithranol	2004028-01	6
Euro OTC	Dithranol	2004028-02	9
Euro OTC	Dithranol	2201006-01	5
Euro OTC	Dithranol	2201006-02	1
Euro OTC	Dithranol	2201006-03	7
Euro OTC	Dithranol	2201006-05	1
Euro OTC	Dithranol	56/11072013	1
Euro OTC	Dithranol	DT/370/2012	1
Euro OTC	Dithranol	DTHX-094	1
Euro/ AHC	Dithranol	2201006-03	1
Euro/ Gehe	Dithranol	APOP-DNL/11/17/002	1
Euro/Jenne	Dithranol	1702022-04	1
Fagron	Dithranol	11L20-N13	1
Fagron	Dithranol	1-21883004	1
Fagron	Dithranol	1218834	1
Fagron	Dithranol	13A30-N01	4
Fagron	Dithranol	17710I-01274	1
Fagron	Dithranol	18823-B50-35511	1
Fagron	Dithranol	18B23-B50-355511	2
Fagron	Dithranol	20C20-B07-200565	1
Fagron	Dithranol	20G27-B01-200443	2
Fagron	Dithranol	20K20-B04	1
Fagron	Dithranol	20K20-B04-203566	1
Fagron	Dithranol	20k20-B04-210534	1
Fagron	Dithranol	20K20-B04-210534	1
Fagron	Dithranol	21/17-B01-213565	1
Fagron	Dithranol	21/17-B01-218834	6
Fagron	Dithranol	21117-801-218834	1
Fagron	Dithranol	21117B01-218834	1
Fagron	Dithranol	21I17-b01-218834	1
Fagron	Dithranol	21I17-B01-218834	4
Fagron	Dithranol	220100603	1
Fagron	Dithranol	22F11-B02-226170	2
Fagron	Dithranol	22F11-BO2-226170	1
Fagron	Dithranol	9K10-N19	1
Fagron	Dithranol	B01-2188304	2
Fagron	Dithranol	BO1-2188304	1
Fagron	Dithranol	OP-DNL-C1-002/21	1
Gehe/Audar	Dithranol	APDT3752012D	1
Gehe/Euro	Dithranol	2201006-03	1
Gehe	Dithranol	1311029-01	1
Gehe	Dithranol	21/17-B01-218834	1
Gehe	Dithranol	22F11-B02-226170	2
Gehe	Dithranol	23F15-B01-231257	1
Gehe	Dithranol	APOP-DNL/11/17/001	1
Jenne / Optimus	Dithranol	2004028-01	1
Jenne	Dithranol	2001025-01	2
jenne	Dithranol	2201006-5	1
Kehr	Dithranol	22F11-B02-226170	1
Kehr	Dithranol	23F15-B01-235539	1
Noweda, EuRho	Dithranol	2201006-03	1
Noweda	Dithranol	1203025-02	1
Noweda	Dithranol	1702022-02	1
Noweda	Dithranol	2201006-04	1
Noweda	Dithranol	22F11-B02-219586	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Dithranol	APDT/375/2012	1
Noweda	Dithranol	DT/375/2012D	1
Optimus Pharma	Dithranol		1
Optimus/Phönix	Dithranol	APOP-DNL11/17/002D	1
Pala	Dithranol	DTHX-097	1
Phoenix/Noweda	Dithranol	APOP-DNL/11/17/002D	1
Phoenix	Dithranol	1701030-01	1
Phoenix	Dithranol	apopdnl11117002d	1
phönix	Dithranol	21000824007	1
Phönix	Dithranol	2201006-05	1
Phönix	Dithranol	Caelo	1
Sanacorp	Dithranol		1
Sanacorp	Dithranol	1702022-04	1
Sanacorp	Dithranol	20K20-B04-210534	1
Sanacorp	Dithranol	21I17B01-213565	1
Sanacorp	Dithranol	22001422005	2
Sanacorp	Dithranol	APDT/375/2012	1
Sanacorp	Dithranol	APOP-DNL/11/17/001-D	1

- 235 501 spectra from 1515 *Apo-Ident* customers from a total of 49 090 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Dithranol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Dithranol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	430	0	152 532
Type B	0	250	0	201 834
Type C	0	525	41	235 501

The substance/substance group *Dithranol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6047 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.6000 %)
Type C	100.0000 % (> 99.9007 %)	92.7562 % (> 92.2261 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24153	24153	0.00	154.98
24169	24169	0.00	148.86
24172	24169	5.47	148.30
24429	24429	0.00	170.57
24501	24501	0.00	146.48
24503	24503	0.00	149.02
25429	25429	0.00	164.43
25502	24153	30.41	144.98
25646	25646	0.00	173.47
25960	25960	0.00	209.55
26452	26452	0.00	151.70

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**DL-Methionine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10004593-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

DL-Methionine; DL-Methioninum

Special notes

When selecting the *DL-Methionine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
DL-Methionine	3	1	2

Second-stage model

For differentiation of the substance/substance group *DL-Methionine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *DL-Methionine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ornithine aspartate	81.85	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *DL-Methionine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *DL-Methionine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	DL-Methionine	172575	25449	40	20171024*
Caelo	DL-Methionine	190211	25450	40	20190306*
Caelo	DL-Methionine	23000413	26714	40	20230323*
Caelo	DL-Methionine	23000413	26714SI	20	20230323*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 140 spectra of 4 reference samples from the substance/substance group *DL-Methionine*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 822 spectra from a total of 2839 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group DL-*Methionine*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	DL-Methionine	193073	25451	40

- 202 044 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group DL-*Methionine*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	DL-Methionine	16274007	1
Caelo	DL-Methionine	21000019005	2

- 236 064 spectra from 1515 *Apo-Ident* customers from a total of 49 256 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *DL-Methionine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *DL-Methionine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	140	0	152 822
Type B	0	40	0	202 044
Type C	0	3	0	236 064

The substance/substance group *DL-Methionine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9011 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25449	25449	0.00	121.24
25450	25450	0.00	117.38
26714	26714	0.00	128.29

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Doxepin hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10005411-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Doxepin hydrochloride; Doxepini hydrochloridum

Special notes

When selecting the *Doxepin hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Doxepin hydrochloride	5	4	0

Second-stage model

For differentiation of the substance/substance group *Doxepin hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Doxepin hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Benzydamine hydrochloride	81.69	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Doxepin hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Doxepin hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Dipharma	Doxepin hydrochloride	1909145	25812	50	20190716
Dipharma	Doxepin hydrochloride	2003479	25814	50	20200312
Dipharma	Doxepin hydrochloride	1909145	25815	50	2204026
Dipharma	Doxepin hydrochloride	2207952	26321	40	20220628
Fagron	Doxepin hydrochloride	18A30-B01-361389	25816	50	20190617
Fagron	Doxepin hydrochloride	21G23-B04-222859	26387	40	20211005

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 6 reference samples from the substance/substance group *Doxepin hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.
- 152 682 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 290 spectra of 13 reference samples from the substance/substance group *Doxepin hydrochloride*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Dipharma	Doxepin hydrochloride	1904946	25813	50
Dipharma	Doxepin hydrochloride	2112869	25897	50
Fagron	Doxepin hydrochloride	20C26-F01-371195	25720	40
Fagron	Doxepin hydrochloride	21G23-B05-215698	25910	40
Dipharma	Doxepin hydrochloride	1909145	25812SI†	10
Dipharma	Doxepin hydrochloride	1904946	25813SI	10
Dipharma	Doxepin hydrochloride	2003479	25814SI†	10
Dipharma	Doxepin hydrochloride	1909145	25815SI†	10
Dipharma	Doxepin hydrochloride	2112869	25897SI	10
Dipharma	Doxepin hydrochloride	2207952	26321SI†	20
Fagron	Doxepin hydrochloride	18A30-B01-361389	25816SI†	10
Fagron	Doxepin hydrochloride	21G23-B05-215698	25910SI	10
Fagron	Doxepin hydrochloride	21G23-B04-222859	26387SI†	20

- 201 794 spectra from a total of 4036 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Doxepin hydrochloride*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Doxepin hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Doxepin hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	290	0	201 794
Type C	0	0	0	236 067

The substance/substance group *Doxepin hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.9310 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25812	25815	12.81	113.88
25814	25815	18.30	127.58
25815	25815	0.00	120.62
25816	25815	13.18	147.47
26321	25815	10.75	111.65
26387	25815	13.63	114.64

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Doxycycline hyclate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20796-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Doxycycline hyclate; Doxycyclini hyclas

Special notes

When selecting the *Doxycycline hyclate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Doxycycline hyclate	6	3	31

Second-stage model

For differentiation of the substance/substance group *Doxycycline hyclate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Doxycycline hyclate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Oxytetracycline hydrochloride	74.46	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Doxycycline hyclate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Doxycycline hyclate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Doxycycline hyclate	12G12-N15	20796	40	1404233
Fagron	Doxycycline hyclate	12G12-N15	20821	40	20120807
Fagron	Doxycycline hyclate	14K28-B05-312218	22242	60	20150216
Fagron	Doxycycline hyclate	19A30-B01-360207	24820	40	20190412
Fagron	Doxycycline hyclate	19I12-F01-366406	24946	40	20191204
Fagron	Doxycycline hyclate	21I10-B02-219301	26328	40	20211117
Fagron	Doxycycline hyclate	21I10-B02-219301	26328SI	20	20211117
Fagron	Doxycycline hyclate	23L01-B01-004244	27469	40	20231219

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 320 spectra of 8 reference samples from the substance/substance group *Doxycycline hyclate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 642 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 5 reference samples from the substance/substance group *Doxycycline hyclate*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Doxycycline hyclate	16I06-B02-330167	23118	40
Fagron	Doxycycline hyclate	18D18-B01-349567	24170	40
Fagron	Doxycycline hyclate	21I15-F01-380126	25905	40
Fagron	Doxycycline hyclate	21I15-F01-380126	25905SI	10
Fagron	Doxycycline hyclate	23L01-B01-004244	27469SI†	20

- 201 934 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 40 spectra from 27 *Apo-Ident* customers from 33 batches from the substance/substance group *Doxycycline hyclate*.
- Among them are spectra of independent samples from 31 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Doxycycline hyclate	2115-F01-380126	1
	Doxycycline hyclate	21I10-B02-221825	1
	Doxycycline hyclate	H202106006	1
AHD	Doxycycline hyclate	18D18-B01-353701	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Doxycycline hyclate	16I06-B02-335675	1
Caelo	Doxycycline hyclate	16I06-B02-341857	1
Fagron	Doxycycline hyclate	12G12-N15	1
Fagron	Doxycycline hyclate	13D24-B40-298948	1
Fagron	Doxycycline hyclate	14K28-B05_312218	1
Fagron	Doxycycline hyclate	14K28-B05-312010	1
Fagron	Doxycycline hyclate	16/06-B02-341857	1
Fagron	Doxycycline hyclate	1603008	1
Fagron	Doxycycline hyclate	1606B02330167	1
Fagron	Doxycycline hyclate	16106-Bo2	1
Fagron	Doxycycline hyclate	16E04-B07-231917	1
Fagron	Doxycycline hyclate	16I06-B02	1
Fagron	Doxycycline hyclate	16I06-B02-330167	1
Fagron	Doxycycline hyclate	16I06-B02-341857	4
Fagron	Doxycycline hyclate	16l06-B02-330167	1
Fagron	Doxycycline hyclate	17112201	1
Fagron	Doxycycline hyclate	18D18_B01_349567	1
Fagron	Doxycycline hyclate	18D18-B01-349567	2
Fagron	Doxycycline hyclate	18D18B01353701	1
Fagron	Doxycycline hyclate	18D18-B01-353701	1
Fagron	Doxycycline hyclate	18D18-B01-353801	1
Fagron	Doxycycline hyclate	19A30-B01	1
Fagron	Doxycycline hyclate	19A30-B01-360207	1
Fagron	Doxycycline hyclate	20101701	1
Fagron	Doxycycline hyclate	20A30-F01-368711	1
Fagron	Doxycycline hyclate	21/10-B02-221825	1
Fagron	Doxycycline hyclate	F01-3687101	1
Fragron/Sanacorp	Doxycycline hyclate	16l06-B02-335675	1
Löwen City-Apotheke …	Doxycycline hyclate	10022014	1
Löwen City-Apotheke …	Doxycycline hyclate	2042015	1
Merck	Doxycycline hyclate	22022019	1
Sanacorp	Doxycycline hyclate	16I06-B02-335675	1

- 236 027 spectra from 1515 *Apo-Ident* customers from a total of 49 226 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Doxycycline hyclate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Doxycycline hyclate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	150	0	201 934
Type C	0	39	1	236 027

The substance/substance group *Doxycycline hyclate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9007 %)	97.5000 % (> 90.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20796	20796	0.00	154.38
20821	20796	9.22	153.01
22242	20796	21.48	154.76
24820	20796	19.13	158.01
24946	20796	17.64	162.00
26328	20796	22.67	154.93
27469	20796	12.71	157.72

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Doxylamine hydrogen succinate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20315-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Doxylamine hydrogen succinate; Doxylamine succinate; Doxylamini hydrogenosuccinas

Special notes

When selecting the *Doxylamine hydrogen succinate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Doxylamine hydrogen succinate	6	6	72

Second-stage model

For differentiation of the substance/substance group *Doxylamine hydrogen succinate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Doxylamine hydrogen succinate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Benzydamine hydrochloride	82.86	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Doxylamine hydrogen succinate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Doxylamine hydrogen succinate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Doxylamine hydrogen succinate	15203906	23085	40	20151112
Caelo	Doxylamine hydrogen succinate	15203906	23086	40	20151112
Caelo	Doxylamine hydrogen succinate	183312	24535	40	20190219*
Fagron	Doxylamine hydrogen succinate	14F03-B01-293498	21542	60	1410524
Fagron	Doxylamine hydrogen succinate	15F01-B04-309189	22601	40	AR-16-FG-011361-01
Fagron	Doxylamine hydrogen succinate	20B19-F06-370985	25518	40	20200320
Fagron	Doxylamine hydrogen succinate	20K05-F03-375371	25838	50	20201207

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 310 spectra of 7 reference samples from the substance/substance group *Doxylamine hydrogen succinate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 652 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 300 spectra of 9 reference samples from the substance/substance group *Doxylamine hydrogen succinate*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Doxylamine hydrogen succinate	172047	23626	40
Caelo	Doxylamine hydrogen succinate	181277	24536	40
Caelo	Doxylamine hydrogen succinate	20002147003	25514	40
Caelo	Doxylamine hydrogen succinate	22000214	26114	40
Caelo	Doxylamine hydrogen succinate	23003003	27119	40
Caelo	Doxylamine hydrogen succinate	24000843	27239	40
Caelo	Doxylamine hydrogen succinate	22000214	26114SI	20
Caelo	Doxylamine hydrogen succinate	23003003	27119SI	20
Caelo	Doxylamine hydrogen succinate	24000843	27239SI	20

- 201 784 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 166 spectra from 32 *Apo-Ident* customers from 74 batches from the substance/substance group *Doxylamine hydrogen succinate*.

- Among them are spectra of independent samples from 68 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Doxylamine hydrogen succinate	B06_2286708	1
Caelo	Doxylamine hydrogen succinate		1
Caelo	Doxylamine hydrogen succinate	14k27-B07	1
Caelo	Doxylamine hydrogen succinate	15F01-B04-317385	2
Caelo	Doxylamine hydrogen succinate	15K04B01327356	1
Caelo	Doxylamine hydrogen succinate	16F06-B02-338804	2
Caelo	Doxylamine hydrogen succinate	16F06-B02-357986	1
Caelo	Doxylamine hydrogen succinate	18331201	1
Caelo	Doxylamine hydrogen succinate	18331206	1
Caelo	Doxylamine hydrogen succinate	21C19-F04-377749	1
Euro OTC	Doxylamine hydrogen succinate	16F06-B02-348869	1
Fagron	Doxylamine hydrogen succinate		5
Fagron	Doxylamine hydrogen succinate	11G20-N10	1
Fagron	Doxylamine hydrogen succinate	11K17-N04	3
Fagron	Doxylamine hydrogen succinate	12811328003	1
Fagron	Doxylamine hydrogen succinate	12811420001	1
Fagron	Doxylamine hydrogen succinate	12811625003	6
Fagron	Doxylamine hydrogen succinate	12E04-N04	3
Fagron	Doxylamine hydrogen succinate	12G10-N03	6
Fagron	Doxylamine hydrogen succinate	12K21-N01	2
Fagron	Doxylamine hydrogen succinate	13/26-N14	1
Fagron	Doxylamine hydrogen succinate	13A04-N02	7
Fagron	Doxylamine hydrogen succinate	13E29-N03	4
Fagron	Doxylamine hydrogen succinate	14F03B01293498	1
Fagron	Doxylamine hydrogen succinate	14F03-B01-296845	1
Fagron	Doxylamine hydrogen succinate	14K27-B07	1
Fagron	Doxylamine hydrogen succinate	14K27-B07-303356	1
Fagron	Doxylamine hydrogen succinate	15F01-B04-308354	1
Fagron	Doxylamine hydrogen succinate	15F01-B04-309189	3
Fagron	Doxylamine hydrogen succinate	15K04-B01	1
Fagron	Doxylamine hydrogen succinate	15K04-B01-317386	1
Fagron	Doxylamine hydrogen succinate	15K04-B01-318794	5
Fagron	Doxylamine hydrogen succinate	15K04-B01-327356	2
Fagron	Doxylamine hydrogen succinate	15k04b01327357	1
Fagron	Doxylamine hydrogen succinate	16F06-B02	2
Fagron	Doxylamine hydrogen succinate	16F06-B-02-338804	1
Fagron	Doxylamine hydrogen succinate	16F06-B02-338805	4
Fagron	Doxylamine hydrogen succinate	16-F06-B02-338805	1
Fagron	Doxylamine hydrogen succinate	16F06-B02-341879	7
Fagron	Doxylamine hydrogen succinate	16F06-B02-348870	2
Fagron	Doxylamine hydrogen succinate	16F-06-B02-348870	1
Fagron	Doxylamine hydrogen succinate	16F-06-B02-3488760	1
Fagron	Doxylamine hydrogen succinate	16F-06-B02-351516	1
Fagron	Doxylamine hydrogen succinate	16F06-B02-353930	3
Fagron	Doxylamine hydrogen succinate	16F06-B02-353931	5
Fagron	Doxylamine hydrogen succinate	16F06-B02-357510	2
Fagron	Doxylamine hydrogen succinate	16F06-B02-357986	2
Fagron	Doxylamine hydrogen succinate	18041818	1
Fagron	Doxylamine hydrogen succinate	19C14-B01	1
Fagron	Doxylamine hydrogen succinate	19C14-B01-362199	2
Fagron	Doxylamine hydrogen succinate	19C14-B01-362200	2
Fagron	Doxylamine hydrogen succinate	19C14-B01-364554	1
Fagron	Doxylamine hydrogen succinate	19C14-B01-364555	2
Fagron	Doxylamine hydrogen succinate	19C14-B01-364557	1
Fagron	Doxylamine hydrogen succinate	19C14-B01-364888	1
Fagron	Doxylamine hydrogen succinate	20B19-F06-368886	2
Fagron	Doxylamine hydrogen succinate	20B19-F06-370985	2
Fagron	Doxylamine hydrogen succinate	20B19-F06-370986	1
Fagron	Doxylamine hydrogen succinate	20B19-F06-370987	1
Fagron	Doxylamine hydrogen succinate	20K05-F03	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Doxylamine hydrogen succinate	21C19-F04-377750	2
Fagron	Doxylamine hydrogen succinate	21C19-F04-377751	1
Fagron	Doxylamine hydrogen succinate	2oko5-F03-375372	1
Fagron	Doxylamine hydrogen succinate	351516	1
Fagron	Doxylamine hydrogen succinate	483875887	1
Fagron	Doxylamine hydrogen succinate	F06-B02-351516/34887	1
L10	Doxylamine hydrogen succinate	16F06B02338805	1
L10	Doxylamine hydrogen succinate	16F06-B02-341879	2
L10	Doxylamine hydrogen succinate	16F06-B02-351516	1
L12	Doxylamine hydrogen succinate	15K04-B01-322165	7
L12	Doxylamine hydrogen succinate	15K04-B01-327357	8
L12	Doxylamine hydrogen succinate	15K04-B01-332765	3
L12	Doxylamine hydrogen succinate	16F06-B02-338805	5
L12	Doxylamine hydrogen succinate	16F06-B02-348870	4
L30	Doxylamine hydrogen succinate	16F06-b02-334258	1
L30	Doxylamine hydrogen succinate	16F06-B02-343936	5

- 235 901 spectra from 1515 *Apo-Ident* customers from a total of 49 184 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Doxylamine hydrogen succinate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Doxylamine hydrogen succinate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	310	0	152 652
Type B	0	300	0	201 784
Type C	0	165	1	235 901

The substance/substance group *Doxylamine hydrogen succinate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0645 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.0000 %)
Type C	100.0000 % (> 99.9007 %)	99.3976 % (> 97.5904 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21542	21542	0.00	122.57
22601	22601	0.00	109.97
23085	24535	21.30	107.14
23086	24535	20.16	107.37
24535	24535	0.00	104.46
25518	22601	29.09	107.22
25838	21542	11.81	113.07

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**EDTA calcium disodium**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10003685-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

EDTA calcium disodium; Natrii calcii edetas; Sodium calcium edetate

Special notes

When selecting the *EDTA calcium disodium* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
EDTA calcium disodium	6	2	3

Second-stage model

For differentiation of the substance/substance group *EDTA calcium disodium* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *EDTA calcium disodium* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Glycerol monostearate, emulsifying	72.86	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *EDTA calcium disodium* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *EDTA calcium disodium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	EDTA calcium disodium	1807024	24145	40	20180725*
Euro OTC	EDTA calcium disodium	1901028	24467	40	20190218*
Euro OTC	EDTA calcium disodium	1910014	24955	40	20191119*
Euro OTC	EDTA calcium disodium	2003032	25242	40	20200527*
Euro OTC	EDTA calcium disodium	2207022	26266	40	20220818*
Euro OTC	EDTA calcium disodium	2207022	26266SI	20	20220818*
Euro OTC	EDTA calcium disodium	2301043	26593	40	20230309*
Euro OTC	EDTA calcium disodium	2301043	26593SI	20	20230309*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 280 spectra of 8 reference samples from the substance/substance group *EDTA calcium disodium*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 682 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 100 spectra of 3 reference samples from the substance/substance group *EDTA calcium disodium*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	EDTA calcium disodium	1705029	23434	40
Euro OTC	EDTA calcium disodium	2311016	27072	40
Euro OTC	EDTA calcium disodium	2311016	27072SI	20

- 201 984 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 1 *Apo-Ident* customers from 4 batches from the substance/substance group *EDTA calcium disodium*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	EDTA calcium disodium	1901028-01Retest	1
Euro OTC	EDTA calcium disodium	1910014-01	1
Euro OTC	EDTA calcium disodium	2003032	1
Euro OTC	EDTA calcium disodium	2010022-01	3

- 236 061 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *EDTA calcium disodium* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *EDTA calcium disodium* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	100	0	201 984
Type C	0	6	0	236 061

The substance/substance group *EDTA calcium disodium* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24145	24145	0.00	182.93
24467	24467	0.00	131.75
24955	24955	0.00	210.47
25242	25242	0.00	176.74
26266	26266	0.00	201.77
26593	26593	0.00	207.26

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Enalapril maleate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10003565-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Enalapril maleate; Enalaprili maleas

Special notes

When selecting the *Enalapril maleate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Enalapril maleate	6	3	12

Second-stage model

For differentiation of the substance/substance group *Enalapril maleate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Enalapril maleate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	102.68	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Enalapril maleate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Enalapril maleate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Enalapril maleate	16K14-B02-336220	23716	40	1801425
Fagron	Enalapril maleate	17J18-B03-347278	24096	40	20171208
Fagron	Enalapril maleate	20F26-F02-372725	25444	40	20200812
Fagron	Enalapril maleate	22F29-B02-223143	26377	40	20220713
Fagron	Enalapril maleate	22F29-B02-223143	26377SI	20	20220713
Fagron	Enalapril maleate	23C23-B01-227968	26683	40	20230427
Fagron	Enalapril maleate	23H22-B08-232432	27031	40	20230919

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 7 reference samples from the substance/substance group *Enalapril maleate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 702 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 170 spectra of 5 reference samples from the substance/substance group *Enalapril maleate*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Enalapril maleate	19H27-F02-364744	24945	40
Fagron	Enalapril maleate	21B19-F03-377278	25840	50
Fagron	Enalapril maleate	21G22-B04-218923	26329	40
Fagron	Enalapril maleate	21G22-B04-218923	26329SI	20
Fagron	Enalapril maleate	23C23-B01-227968	26683SI†	20

- 201 914 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 38 spectra from 28 *Apo-Ident* customers from 15 batches from the substance/substance group *Enalapril maleate*.
- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Enalapril maleate	21G22-B04-218923	1
	Enalapril maleate	23C23-B01-227968	2
Fagron	Enalapril maleate	19H27-F02-364744	2
Fagron	Enalapril maleate	1G22-B04-218923	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Enalapril maleate	20F26-F02	1
Fagron	Enalapril maleate	20F26-F02-372725	12
Fagron	Enalapril maleate	21B19-F03-3772708	1
Fagron	Enalapril maleate	21B19-F03-377278	5
Fagron	Enalapril maleate	21G22-B04	2
Fagron	Enalapril maleate	21G22-B04-218923	3
Fagron	Enalapril maleate	22F29-B02-223143	1
Fagron	Enalapril maleate	2OF26-F02-372725	1
Fagron	Enalapril maleate	3012-2004-008	1
Fagron	Enalapril maleate	811-01000	1
Fagron	Enalapril maleate	F02-3272005	1
Jenne	Enalapril maleate	23C23-B01-227968	1
Nachprüfung	Enalapril maleate	AP200615-11	1
Noweda	Enalapril maleate	22F29-B02-223143	1

- 236 029 spectra from 1515 *Apo-Ident* customers from a total of 49 243 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Enalapril maleate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Enalapril maleate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	170	0	201 914
Type C	0	38	0	236 029

The substance/substance group *Enalapril maleate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.4706 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 84.2105 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23716	23716	0.00	222.19
24096	23716	6.67	228.49
25444	23716	10.96	222.78
26377	23716	9.08	222.98
26683	23716	11.60	221.50
27031	23716	18.39	228.64

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Eosin Y**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20571-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Eosin Y; Eosinum natricum

Special notes

When selecting the *Eosin Y* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Eosin Y	7	3	58

Second-stage model

For differentiation of the substance/substance group *Eosin Y* the following second-stage model is used:

- Submodel 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Eosin Y* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	58.88	–
⋮	⋮	⋮
Dequalinium chloride	>50	58.19
Levothyroxin sodium	>50	62.34
Oxytetracycline hydrochloride	>50	91.58
Tannin	>50	127.44
Sodium salicylate	>50	276.47
Dithranol	>50	302.29
Acetylsalicylic acid	>50	341.36
Benzoic acid	>50	380.65

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Eosin Y* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Eosin Y*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Eosin Y	12E25-N01	20900	60	20120607
Fagron	Eosin Y	15G01-T03-025958	22261	60	1604114
Fagron	Eosin Y	13F14-T01-017395	22534	40	1608469
Fagron	Eosin Y	13F14-T01-017395	22535	40	20141219
Fagron	Eosin Y	13F14-T01-017395	22660	40	1801115
Fagron	Eosin Y	13F14-T01-017395	22816	40	1705197
Fagron	Eosin Y	17K21-T07-042542	23975	40	1805338
Fagron	Eosin Y	19J25-B06-196532	25187	40	20191216
Fagron	Eosin Y	20G07-B02-200510	25503	40	20200730
Fagron	Eosin Y	23E10-B02-228749	26822	40	20230619

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 440 spectra of 10 reference samples from the substance/substance group *Eosin Y*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 522 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 6 reference samples from the substance/substance group *Eosin Y*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Eosin Y	13I11-N03	20932	40
Fagron	Eosin Y	20J13-B01-201856	25754	40
Fagron	Eosin Y	21L20-B06-213987	26063	40
Fagron	Eosin Y	13I11-N03	21208	40
Fagron	Eosin Y	21L20-B06-213987	26063SI	20
Fagron	Eosin Y	23E10-B02-228749	26822SI†	20

- 201 884 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 200 spectra from 170 *Apo-Ident* customers from 69 batches from the substance/substance group *Eosin Y*.

- Among them are spectra of independent samples from 58 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Eosin Y	21L20-B06	1
	Eosin Y	21L20-B06-213987	1
	Eosin Y	22I27-B01-223849	4
	Eosin Y	22I27-B01-223850	1
	Eosin Y	23E10-B02-228749	2
	Eosin Y	B06-2139807	2
	Eosin Y	EYWS/03/22	1
Cael Sanacorp 05.02.2016	Eosin Y	13F14-T01-017395	1
Caelo	Eosin Y	12e25n01	1
Caelo	Eosin Y	12e25-n01	1
Caelo	Eosin Y	13F14-T01-017395	1
Caelo	Eosin Y	13I11-N03	1
Caelo	Eosin Y	14H28-M05	1
Caelo	Eosin Y	15G01-T03-025958	1
Caelo	Eosin Y	17K21-T07	1
Caelo	Eosin Y	20J13-BO1-201856	1
Fagron	Eosin Y	1(20G0-B02-200510)	1
Fagron	Eosin Y	11E25-N01	1
Fagron	Eosin Y	11F21-N10	1
Fagron	Eosin Y	12A02-N09	2
Fagron	Eosin Y	12E25-N01	4
Fagron	Eosin Y	12H28-N08	3
Fagron	Eosin Y	13/11-N03	3
Fagron	Eosin Y	13/11-NO3	1
Fagron	Eosin Y	13F14-T01-017395	6
Fagron	Eosin Y	13fF14-T01-017395	1
Fagron	Eosin Y	14H28-M05	4
Fagron	Eosin Y	14H28-M09	2
Fagron	Eosin Y	15G01-T03	1
Fagron	Eosin Y	15G01-T03-025958	5
Fagron	Eosin Y	15G01T03025959	1
Fagron	Eosin Y	15G01-T03-027933	2
Fagron	Eosin Y	15G01-T03-034438	1
Fagron	Eosin Y	17372-87-1	2
Fagron	Eosin Y	17K21-T0-054710	1
Fagron	Eosin Y	17K21-T07	4
Fagron	Eosin Y	17K21-T07_062160	1
Fagron	Eosin Y	17K21-T07-042542	4
Fagron	Eosin Y	17K21T07-054710	1
Fagron	Eosin Y	17K21-T07-054710	9
Fagron	Eosin Y	17K21-T07-057542	4
Fagron	Eosin Y	17K21-T07-057543	1
Fagron	Eosin Y	17K21T07060102	1
Fagron	Eosin Y	17K21-T07-060102	7
Fagron	Eosin Y	17K21-T07-060103	1
Fagron	Eosin Y	17K21-T07-062160	14
Fagron	Eosin Y	19j25-b06-196532	2
Fagron	Eosin Y	19J25-B06-196532	10
Fagron	Eosin Y	201856	1
Fagron	Eosin Y	20g07-b02-200510	1
Fagron	Eosin Y	20G07-B02-200510	7
Fagron	Eosin Y	20G07-B02-200567	1
Fagron	Eosin Y	20J13_B01_201856	1
Fagron	Eosin Y	20J13-B01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Eosin Y	20J13-B01-201856	19
Fagron	Eosin Y	20J13-B01	1
Fagron	Eosin Y	20J13-B01-201856	1
Fagron	Eosin Y	21L20-B06	1
Fagron	Eosin Y	21L20-B06-213987	7
Fagron	Eosin Y	2200510	1
Fagron	Eosin Y	54710	1
Fagron	Eosin Y	701074-0001	1
Fagron	Eosin Y	B01-2018506	1
Fagron	Eosin Y	B06-1965302	5
Fagron	Eosin Y	EYWS/02/20	1
Fagron	Eosin Y	EYWS/09/17	1
Fagron	Eosin Y	EYWS/12/19	2
Fagron	Eosin Y	EYWS/15/13	1
Fagron	Eosin Y	EYWS/16/11	2
Fagron	Eosin Y	EYWS/16/9	1
Fagron	Eosin Y	T07-0621600	1
Fargon/noweda	Eosin Y	21L20-B06-213987	1
Fargon/Sanacorp	Eosin Y	13/11-No3	1
Fargon	Eosin Y	19J25-B06-196532	2
Fiebig	Eosin Y	13F14-T01-017395	1
Fiebig	Eosin Y	EYWS/16/19	1
Gehe	Eosin Y	14H28-M05	1
Gehe	Eosin Y	19j25-b06-196532	1
Gehe	Eosin Y	20J13-B01-201856	1
Gilbert/Gehe	Eosin Y	1K21-T07-062160	1
JPN Pharma Pvt Ltd	Eosin Y	21L20-B06	1
L12	Eosin Y	17K21-T07-054710	1
Noweda	Eosin Y	20J13B01201856	1
Noweda	Eosin Y	21L20-B06	1
Sanacorp	Eosin Y	12E25-N01	1
sanacorp	Eosin Y	14H28-M05	1
Sanacorp	Eosin Y	22127-B01-223849	1
Sanacorp	Eosin Y	T07-0621600	1

- 235 867 spectra from 1515 *Apo-Ident* customers from a total of 49 189 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Eosin Y* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Eosin Y* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	200	0	201 884
Type C	0	196	4	235 867

The substance/substance group *Eosin Y* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9007 %)	98.0000 % (> 96.5000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20900	22534	57.15	187.44
22261	22261	0.00	160.87
22534	22534	0.00	152.40
22535	22660	2.20	216.27
22660	22660	0.00	217.06
22816	22816	0.00	214.49
23975	23975	0.00	165.26
25187	22660	44.99	192.94
25503	22660	76.40	206.07
26822	22534	116.61	187.39

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ephedrine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20993-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ephedrine hydrochloride; Ephedrini hydrochloridum

Special notes

When selecting the *Ephedrine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ephedrine hydrochloride	6	4	67

Second-stage model

For differentiation of the substance/substance group *Ephedrine hydrochloride* the following second-stage model is used:

- Submodel 08

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ephedrine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	149.40	–
⋮	⋮	⋮
Prednisone	>50	33.07
Prednisolone acetate	>50	51.44

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ephedrine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ephedrine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ephedrine hydrochloride	12017217	20993	40	1511635
Caelo	Ephedrine hydrochloride	13323305	21322	40	20131113
Caelo	Ephedrine hydrochloride	14378502	21803	60	20150106
Caelo	Ephedrine hydrochloride	161197	22436	60	20160420*
Caelo	Ephedrine hydrochloride	21000335008	25729	40	20210125
Caelo	Ephedrine hydrochloride	21000335008	25729SI	40	20210125
Fagron	Ephedrine hydrochloride	15H28-B02-316349	23073	40	20150924

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 320 spectra of 7 reference samples from the substance/substance group *Ephedrine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 250 spectra of 7 reference samples from the substance/substance group *Ephedrine hydrochloride*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ephedrine hydrochloride	171736	23672	40
Caelo	Ephedrine hydrochloride	22001784	26372	40
Caelo	Ephedrine hydrochloride	23001657	26841	30
Fagron	Ephedrine hydrochloride	20H07-B01-202226	25970	40
Caelo	Ephedrine hydrochloride	22001784	26372SI	30
Caelo	Ephedrine hydrochloride	23001657	26841SI	30
Fagron	Ephedrine hydrochloride	20H07-B01-202226	25970SI	40

- 201 834 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 133 spectra from 52 *Apo-Ident* customers from 71 batches from the substance/substance group *Ephedrine hydrochloride*.

- Among them are spectra of independent samples from 67 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Anzag	Ephedrine hydrochloride	18213113	1
Caelo	Ephedrine hydrochloride		1
Caelo	Ephedrine hydrochloride	10103425	1
Caelo	Ephedrine hydrochloride	10119709	1
Caelo	Ephedrine hydrochloride	11126407	1
Caelo	Ephedrine hydrochloride	12017207	1
Caelo	Ephedrine hydrochloride	12017209	2
Caelo	Ephedrine hydrochloride	12017215	1
Caelo	Ephedrine hydrochloride	12017217	1
Caelo	Ephedrine hydrochloride	12017223	1
Caelo	Ephedrine hydrochloride	13323302	1
Caelo	Ephedrine hydrochloride	13323310	1
Caelo	Ephedrine hydrochloride	13323316	1
Caelo	Ephedrine hydrochloride	13323321	1
Caelo	Ephedrine hydrochloride	14378502	1
Caelo	Ephedrine hydrochloride	14378506	2
Caelo	Ephedrine hydrochloride	14378507	1
Caelo	Ephedrine hydrochloride	14378508	1
Caelo	Ephedrine hydrochloride	14378510	1
Caelo	Ephedrine hydrochloride	15179302	2
Caelo	Ephedrine hydrochloride	151J9304	1
Caelo	Ephedrine hydrochloride	16119702	3
Caelo	Ephedrine hydrochloride	16119703	1
Caelo	Ephedrine hydrochloride	16119704	1
Caelo	Ephedrine hydrochloride	16119709	2
Caelo	Ephedrine hydrochloride	16119710	1
Caelo	Ephedrine hydrochloride	16119715	5
Caelo	Ephedrine hydrochloride	16119715200218P301	1
Caelo	Ephedrine hydrochloride	1619704	1
Caelo	Ephedrine hydrochloride	1713601	1
Caelo	Ephedrine hydrochloride	17173601	1
Caelo	Ephedrine hydrochloride	17173604	1
Caelo	Ephedrine hydrochloride	18006701	4
Caelo	Ephedrine hydrochloride	18006702	1
Caelo	Ephedrine hydrochloride	18006708	1
Caelo	Ephedrine hydrochloride	18006709	1
Caelo	Ephedrine hydrochloride	1813113	1
Caelo	Ephedrine hydrochloride	1821	1
Caelo	Ephedrine hydrochloride	182131002	1
Caelo	Ephedrine hydrochloride	182131003	6
Caelo	Ephedrine hydrochloride	18213103	6
Caelo	Ephedrine hydrochloride	18213104	2
Caelo	Ephedrine hydrochloride	18213105	1
Caelo	Ephedrine hydrochloride	18213109	2
Caelo	Ephedrine hydrochloride	18213111	1
Caelo	Ephedrine hydrochloride	18213112	1
Caelo	Ephedrine hydrochloride	18213113	2
Caelo	Ephedrine hydrochloride	18213115	6
Caelo	Ephedrine hydrochloride	192679004	2
Caelo	Ephedrine hydrochloride	21000335002	1
Caelo	Ephedrine hydrochloride	21000335004	3
Caelo	Ephedrine hydrochloride	21000335009	1
Caelo	Ephedrine hydrochloride	21000335011	1
Caelo	Ephedrine hydrochloride	21000335012	2
Caelo	Ephedrine hydrochloride	21000335013	1
Caelo	Ephedrine hydrochloride	22001784007	1
Caesar & Loretz GmbH...	Ephedrine hydrochloride	11126411	1
Caesar & Loretz GmbH	Ephedrine hydrochloride	14378503	1
Caesar & Loretz GmbH	Ephedrine hydrochloride	18213103	1
Caesar & Loretz GmbH	Ephedrine hydrochloride	18213104	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Ephedrine hydrochloride	18213109	1
Caesar & Loretz GmbH	Ephedrine hydrochloride	18213113	3
Caesar & Loretz GmbH	Ephedrine hydrochloride	18213115	2
Caesar & Loretz GmbH	Ephedrine hydrochloride	192679004	2
Caesar & Loretz GmbH	Ephedrine hydrochloride	21000335002	1
Caesar & Loretz GmbH	Ephedrine hydrochloride	21000335011	3
Caesar & Loretz GmbH	Ephedrine hydrochloride	21000335012	2
Caesar & Loretz GmbH	Ephedrine hydrochloride	22001784003	1
Caesar & Loretz GmbH	Ephedrine hydrochloride	22001784011	2
Caesar & Loretz Hilden	Ephedrine hydrochloride	18213103	1
Cealo, GEHE	Ephedrine hydrochloride	21000335001	1
Fagron	Ephedrine hydrochloride	12017220	1
Fagron	Ephedrine hydrochloride	13B19-N04	1
Fagron	Ephedrine hydrochloride	13L30-B36	1
Gatt-Koller / Phoenix	Ephedrine hydrochloride	18502141114	1
GATT-KOLLER/PHOENIX	Ephedrine hydrochloride	915/03141314	2
Gehe am 04.03.14	Ephedrine hydrochloride	13323303	1
LandSiegfried Pharma…	Ephedrine hydrochloride	17242077	5
LandSiegfried Pharma…	Ephedrine hydrochloride	19212002	1
Phoenix 04.03.14	Ephedrine hydrochloride	1332303	1
PHOENIX 10.03.2014	Ephedrine hydrochloride	13323302	1
Phönix	Ephedrine hydrochloride	13323305	2
Phönix	Ephedrine hydrochloride	13323315	1

- 235 934 spectra from 1515 *Apo-Ident* customers from a total of 49 188 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ephedrine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ephedrine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	210	40	201 834
Type C	0	133	0	235 934

The substance/substance group *Ephedrine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	84.0000 % (> 82.8000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 95.4887 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20993	20993	0.00	214.97
21322	22436	7.50	212.83
21803	22436	4.79	213.76
22436	22436	0.00	216.41
23073	20993	5.33	214.41
25729	22436	5.88	212.80

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Epinephrine hydrogen tartrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20689-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Epinephrine hydrogen tartrate; Adrenaline hydrogen tartrate; Adrenalini tartras

Special notes

When selecting the *Epinephrine hydrogen tartrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Epinephrine hydrogen tartrate	7	5	34

Second-stage model

For differentiation of the substance/substance group *Epinephrine hydrogen tartrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Epinephrine hydrogen tartrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	100.16	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Epinephrine hydrogen tartrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Epinephrine hydrogen tartrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Epinephrine hydrogen tartrate	12120202	20689	40	1405614
Caelo	Epinephrine hydrogen tartrate	12337804	21058	40	20121128
Caelo	Epinephrine hydrogen tartrate	14007802	21489	60	1603180
Caelo	Epinephrine hydrogen tartrate	14007802	21489SI	60	1603180
Caelo	Epinephrine hydrogen tartrate	14007802	21490	60	20140130
Caelo	Epinephrine hydrogen tartrate	14007802	21491	20	20140130
Caelo	Epinephrine hydrogen tartrate	14007802	21492	20	20140130
Caelo	Epinephrine hydrogen tartrate	14007802	21493	20	20140130
Caelo	Epinephrine hydrogen tartrate	14007802	21494	60	20140130
Caelo	Epinephrine hydrogen tartrate	14007802	21495	20	20140130
Caelo	Epinephrine hydrogen tartrate	14007802	21496	20	20140130
Caelo	Epinephrine hydrogen tartrate	14007802	21497	20	20140130
Caelo	Epinephrine hydrogen tartrate	14007802	21498	20	20140130
Caelo	Epinephrine hydrogen tartrate	20004277006	25728	40	20201214
Caelo	Epinephrine hydrogen tartrate	20004277006	25728SI	40	20201214
Caelo	Epinephrine hydrogen tartrate	21004241	26299	40	20220622*
Caelo	Epinephrine hydrogen tartrate	21004241	26299SI	40	20220622*
Fagron	Epinephrine hydrogen tartrate	12L22-N04	20749	40	20120106
Fagron	Epinephrine hydrogen tartrate	18K30-B03-358514	24706	40	20190320

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 700 spectra of 19 reference samples from the substance/substance group *Epinephrine hydrogen tartrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 262 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 720 spectra of 21 reference samples from the substance/substance group *Epinephrine hydrogen tartrate*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Epinephrine hydrogen tartrate	162764	22777	40
Caelo	Epinephrine hydrogen tartrate	171115	23323	40
Caelo	Epinephrine hydrogen tartrate	181795	24260	40
Caelo	Epinephrine hydrogen tartrate	22002542002	26553	40
Caelo	Epinephrine hydrogen tartrate	24000754	27466	40
Caelo	Epinephrine hydrogen tartrate	14007802	21490SI†	60
Caelo	Epinephrine hydrogen tartrate	14007802	21491SI†	20
Caelo	Epinephrine hydrogen tartrate	14007802	21492SI†	20
Caelo	Epinephrine hydrogen tartrate	14007802	21493SI†	20
Caelo	Epinephrine hydrogen tartrate	14007802	21495SI†	20
Caelo	Epinephrine hydrogen tartrate	14007802	21496SI†	20
Caelo	Epinephrine hydrogen tartrate	14007802	21497SI†	20
Caelo	Epinephrine hydrogen tartrate	14007802	21498SI†	20
Caelo	Epinephrine hydrogen tartrate	162764	22777SI	40
Caelo	Epinephrine hydrogen tartrate	171115	23323SI	40
Caelo	Epinephrine hydrogen tartrate	171115	23326	40
Caelo	Epinephrine hydrogen tartrate	171115	23326SI	40
Caelo	Epinephrine hydrogen tartrate	181795	24260SI	40
Caelo	Epinephrine hydrogen tartrate	22002542002	26553SI	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Epinephrine hydrogen tartrate	24000754	27466SI	40
Fagron	Epinephrine hydrogen tartrate	18K30-B03-358514	24706SI[†]	40

- 201 364 spectra from a total of 4038 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 68 spectra from 37 *Apo-Ident* customers from 38 batches from the substance/substance group *Epinephrine hydrogen tartrate*.

- Among them are spectra of independent samples from 33 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
AHD 17.11.14 EK 7,60	Epinephrine hydrogen tartrate		1
Alliance Health 12.03.14	Epinephrine hydrogen tartrate	12337805	1
Caelo	Epinephrine hydrogen tartrate	10237109	1
Caelo	Epinephrine hydrogen tartrate	12120202	1
Caelo	Epinephrine hydrogen tartrate	123337805	1
Caelo	Epinephrine hydrogen tartrate	12337801	1
Caelo	Epinephrine hydrogen tartrate	12337805	2
Caelo	Epinephrine hydrogen tartrate	14007808	1
Caelo	Epinephrine hydrogen tartrate	14301002	2
Caelo	Epinephrine hydrogen tartrate	15194102	2
Caelo	Epinephrine hydrogen tartrate	15194104	1
Caelo	Epinephrine hydrogen tartrate	15239701	2
Caelo	Epinephrine hydrogen tartrate	15239703	1
Caelo	Epinephrine hydrogen tartrate	162746402	1
Caelo	Epinephrine hydrogen tartrate	16276402	2
Caelo	Epinephrine hydrogen tartrate	16276406	2
Caelo	Epinephrine hydrogen tartrate	17111503	3
Caelo	Epinephrine hydrogen tartrate	181795003	1
Caelo	Epinephrine hydrogen tartrate	18179503	2
Caelo	Epinephrine hydrogen tartrate	18179504	5
Caelo	Epinephrine hydrogen tartrate	18179505	2
Caelo	Epinephrine hydrogen tartrate	20004277006	1
Caelo	Epinephrine hydrogen tartrate	210316-1	1
Caelo	Epinephrine hydrogen tartrate	210316-3	1
Caelo	Epinephrine hydrogen tartrate	22002542002	2
Caesar & Loretz GmbH...	Epinephrine hydrogen tartrate	20004277006	1
Caesar & Loretz GmbH	Epinephrine hydrogen tartrate	18179505	1
Caesar & Loretz GmbH	Epinephrine hydrogen tartrate	20004277006	2
Caesar & Loretz GmbH	Epinephrine hydrogen tartrate	22002542002	1
Fagron	Epinephrine hydrogen tartrate	12/02-N03	1
Fagron	Epinephrine hydrogen tartrate	12011902	1
Fagron	Epinephrine hydrogen tartrate	12G11-N07	1
Fagron	Epinephrine hydrogen tartrate	12G11-No70076/130	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Epinephrine hydrogen tartrate	13I04-N03	1
Fagron	Epinephrine hydrogen tartrate	13I04-N03	1
Fagron	Epinephrine hydrogen tartrate	14E12-B02	1
Fagron	Epinephrine hydrogen tartrate	15A13-B02-305559	2
Fagron	Epinephrine hydrogen tartrate	16e09-b11-319882	1
Fagron	Epinephrine hydrogen tartrate	16E09-B11-319882	4
Fagron	Epinephrine hydrogen tartrate	E80-18002	4
Fagron	Epinephrine hydrogen tartrate	E80-18002	1
Gehe	Epinephrine hydrogen tartrate	17111503	1
GEHE	Epinephrine hydrogen tartrate	18179504	1
Phoenix 22.5.14	Epinephrine hydrogen tartrate	12337804	1
Wuhan/Noweda	Epinephrine hydrogen tartrate	C38-190902	1

- 235 999 spectra from 1515 *Apo-Ident* customers from a total of 49 220 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Epinephrine hydrogen tartrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Epinephrine hydrogen tartrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	700	0	152 262
Type B	0	720	0	201 364
Type C	0	68	0	235 999

The substance/substance group *Epinephrine hydrogen tartrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1429 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.1667 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 91.1765 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20689	20689	0.00	235.16
20749	21489	18.60	230.38
21058	20689	5.20	235.13
21489	21489	0.00	247.01
21490	21489	5.01	258.96
21491	21489	2.92	246.66
21492	21489	6.41	231.24
21493	21489	2.24	244.01
21494	21489	9.45	241.82
21495	21489	3.91	246.94
21496	21489	6.58	234.44
21497	20689	8.79	231.07
21498	21489	2.98	245.77
24706	20689	6.52	238.21
25728	21489	9.09	243.87
26299	26299	0.00	236.42

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Erythromycin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20011-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Erythromycin; Erythromycinum

Special notes

When selecting the *Erythromycin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Erythromycin	9	17	908

Second-stage model

For differentiation of the substance/substance group *Erythromycin* the following second-stage model is used:

- Submodel 07

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Erythromycin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prednisolon dihydrogen phosphate di…	76.24	–
⋮	⋮	⋮
Budesonide	>50	16.44
Betamethasone valerate	>50	19.99

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Erythromycin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Erythromycin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Erythromycin	13175601	21323	40	20130620
Caelo	Erythromycin	160792	22438	60	20160408*
Euro OTC	Erythromycin	1308016-02	21651	60	1412542
Euro OTC	Erythromycin	1508034	21890	60	20150925*
Euro OTC	Erythromycin	1607038	22832	40	20160831*
Euro OTC	Erythromycin	1705038	23438	40	20170705*
Euro OTC	Erythromycin	1811019	24420	40	20190114*
Fagron	Erythromycin	12E24-N04	21056	60	20120607
Fagron	Erythromycin	14B06-B35-290872	21669	60	20140225

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 460 spectra of 9 reference samples from the substance/substance group *Erythromycin*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 502 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 840 spectra of 21 reference samples from the substance/substance group *Erythromycin*.

- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Erythromycin	160795	22439	60
Caelo	Erythromycin	160797	22440	60
Caelo	Erythromycin	160796	22442	60
Caelo	Erythromycin	21002046	25858	50
Caelo	Erythromycin	21002044	25859	50
Caelo	Erythromycin	22001550	26629	40
Euro OTC	Erythromycin	1906032	24781	40
Euro OTC	Erythromycin	2002018	25121	40
Euro OTC	Erythromycin	2002038	25123	40
Euro OTC	Erythromycin	2007017	25432	40
Euro OTC	Erythromycin	2010015	25574	40
Euro OTC	Erythromycin	2010014	25575	40
Euro OTC	Erythromycin	2206001	26206	40
Euro OTC	Erythromycin	2301053	26602	40
Euro OTC	Erythromycin	2308010	26940	40
Euro OTC	Erythromycin	2407014	27369	40
Fagron	Erythromycin	23D27-B01-227928	26824	40
Caelo	Erythromycin	22001550	26629SI	20
Euro OTC	Erythromycin	2206001	26206SI	20
Euro OTC	Erythromycin	2301053	26602SI	20
Euro OTC	Erythromycin	2407014	27369SI	20

- 201 244 spectra from a total of 4028 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6320 spectra from 1306 *Apo-Ident* customers from 956 batches from the substance/substance group *Erythromycin*.

- Among them are spectra of independent samples from 905 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Erythromycin		1
	Erythromycin	1308016-02	1
	Erythromycin	2007017-01	2
	Erythromycin	2010015-03	1
	Erythromycin	21/13-B02-213864	1
	Erythromycin	21002041006	1
	Erythromycin	21002041007	1
	Erythromycin	21002041009	1
	Erythromycin	21002041010	3
	Erythromycin	21002041011	2
	Erythromycin	21002041014	3
	Erythromycin	21002042001	1
	Erythromycin	21002053002	6
	Erythromycin	2113-B02-213864	1
	Erythromycin	21A26-F01-376732	3
	Erythromycin	21F02-F02-379295	1
	Erythromycin	21I13-B02-213865	5
	Erythromycin	21l13-B02-213865	1
	Erythromycin	22001550001	3
	Erythromycin	22001550002	7
	Erythromycin	22001550003	5
	Erythromycin	22001550005	10
	Erythromycin	22002199001	7
	Erythromycin	22002199002	7
	Erythromycin	22002199003	2
	Erythromycin	22002200001	2
	Erythromycin	22002200002	3
	Erythromycin	22002200003	3
	Erythromycin	22002200004	9
	Erythromycin	22002200005	4
	Erythromycin	22002202003	6
	Erythromycin	22002203001	1
	Erythromycin	2206001-01	13
	Erythromycin	2208001-01	1
	Erythromycin	221/13-B02-213770	1
	Erythromycin	2-21386004	1
	Erythromycin	22C2200P	1
	Erythromycin	22C2300P	1
	Erythromycin	22C230P	2
	Erythromycin	23003351002	1
	Erythromycin	23003387001	1
	Erythromycin	23003387002	1
	Erythromycin	2301052-02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Erythromycin	230105301	1
	Erythromycin	2301053-01	26
	Erythromycin	2301053-02	11
	Erythromycin	2308010-01	5
	Erythromycin	23d27_b01_227795	1
	Erythromycin	23D27-B01-227795	1
	Erythromycin	23D27-B01-227928	2
	Erythromycin	23D27-B01-227929	7
	Erythromycin	23D27-B01-227930	1
	Erythromycin	23H23-B04-231446	2
	Erythromycin	324464	1
	Erythromycin	4H21P	2
	Erythromycin	A000586(Campus)	1
	Erythromycin	B01-2277905	1
	Erythromycin	B01-2279300	2
	Erythromycin	B01-2279301	1
	Erythromycin	B34-0011103	1
	Erythromycin	CEPEB004H21P	1
	Erythromycin	CEPEB022C22P	1
,0+	Erythromycin	180964001	1
AbZ	Erythromycin	18F05-B01-350908	1
AHC 04.07.13 EK38,50	Erythromycin	12156207	1
AHD 26.02.16 13,15EUR	Erythromycin	14I30-B01-308789	1
AHD/EuRho	Erythromycin	1906032-01	1
AHD	Erythromycin	1409019-02	1
AHD	Erythromycin	180964005	1
AHD	Erythromycin	18110119-01	1
AHD	Erythromycin	21002041002	1
AHD	Erythromycin	22001550002	1
AHD	Erythromycin	22002199001	2
AHD	Erythromycin	22002200005	2
AHD	Erythromycin	2301053-01	1
AHD	Erythromycin	2301053-02	1
AHD	Erythromycin	2308010-01	1
AlH	Erythromycin	15042902	1
Alliance Health	Erythromycin	120503502	1
Alliance Healthcare	Erythromycin	12E24-N04	1
Alliance Healthcare	Erythromycin	13F12-N21	1
Alliance Healthcare	Erythromycin	1607038-02	1
Alliance healthcare	Erythromycin	20003732007	1
Alliance Healthcare	Erythromycin	20E18-F06-371571	1
Alliance Healthcare	Erythromycin	21002041006	1
Alliance Healthcare	Erythromycin	21A26-F01-376731	5
Alliance Healthcare	Erythromycin	22002200004	1
Alliance Healthcare	Erythromycin	CEPEB003D20P	1
Alliance	Erythromycin	22001550002	1
Alliance	Erythromycin	2206001-01	1
alliance	Erythromycin	2301053-01	1
Allianz Healthcare	Erythromycin	16079602	1
Allianz Healthcare	Erythromycin	1811019-02	1
Alte Apotheke	Erythromycin	16079206	1
Anuh Pharma Itd (site)	Erythromycin	20I07-F06-375516	1
Anuh Pharma Itd/ AHD	Erythromycin	19C21-B03-361400	1
Anuh Pharma Itd/ AHD	Erythromycin	19C21-B03-361725	1
Anuh Pharma Itd/ AHD	Erythromycin	19C-B03-361400	1
Anuh Pharma/Sanacorp	Erythromycin	19L18-F02-3677709	1
Anuh Pharma	Erythromycin	18Fo5-B01-354817	1
Anzag 23.11.12 ek:26,49	Erythromycin	1205035-01	1
Anzag	Erythromycin	12152206	1
Anzag	Erythromycin	13175506	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Anzag	Erythromycin	14044001	1
Anzag	Erythromycin	16079501	1
Anzag	Erythromycin	2010014-01	1
Anzag	Erythromycin	22002199001	1
Apo-Ident / Phoenix	Erythromycin	EBS/1701-BM-001	1
Apoident/ Phoenix	Erythromycin	1906032-01	1
apo-ident/Alliance	Erythromycin	2007017-01	1
apo-ident/GEHE	Erythromycin	1607038-01	4
apo-ident/Phoenix	Erythromycin	190292002	1
apo-ident/Phönix	Erythromycin	2010014-01	1
apo-ident/Phönix	Erythromycin	2010015-01	1
apo-ident	Erythromycin	1607038-01	1
apo-ident	Erythromycin	1607038-02	1
apo-ident	Erythromycin	1705038-01	1
Audor Pharma	Erythromycin	13175602	1
Audor Pharma	Erythromycin	2002018-01	1
Audor Pharma	Erythromycin	2010015-01	1
Audor Pharma	Erythromycin	APEB022/17E	1
Audor Pharma	Erythromycin	APEB022I17E	1
Audor Pharma	Erythromycin	EB022I17E	1
Biomed / Gehe	Erythromycin	1508034-01	1
Biomed / Gehe	Erythromycin	1508034-02	1
Biomed / Gehe	Erythromycin	1705038-03	1
Biomed/Phönix	Erythromycin	1607038-01	1
Biomed	Erythromycin	1508035-01	1
Bionorica Ethics	Erythromycin	1906032-01EBS/19-022	1
Bombastus	Erythromycin	14B06-B35-290873	1
Bombastus	Erythromycin	14F13-B02	1
Bombastus	Erythromycin	15042603	1
Bombastus	Erythromycin	16079606	1
Bombastus	Erythromycin	1705038-03	1
Bombastus	Erythromycin	17088402	1
Caelo	Erythromycin		4
Caelo	Erythromycin	10079203	1
Caelo	Erythromycin	1008018-02	1
Caelo	Erythromycin	10091502	1
Caelo	Erythromycin	10788402	1
Caelo	Erythromycin	10896403	1
Caelo	Erythromycin	1091801	1
Caelo	Erythromycin	1102024-01	1
Caelo	Erythromycin	11092001	1
Caelo	Erythromycin	1114Q-01362	1
Caelo	Erythromycin	11195306	1
Caelo	Erythromycin	11195402	3
Caelo	Erythromycin	11195405	1
Caelo	Erythromycin	11195407	3
Caelo	Erythromycin	11195408	1
Caelo	Erythromycin	1171116	1
Caelo	Erythromycin	1181116	1
Caelo	Erythromycin	1195407	1
Caelo	Erythromycin	11j06-n05	1
Caelo	Erythromycin	1205036-01	2
Caelo	Erythromycin	12051801	1
Caelo	Erythromycin	12152101	3
Caelo	Erythromycin	12152102	3
Caelo	Erythromycin	12152104	2
Caelo	Erythromycin	12152105	3
Caelo	Erythromycin	12152107	1
Caelo	Erythromycin	12152108	3
Caelo	Erythromycin	12152109	10

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Erythromycin	1215219	1
Caelo	Erythromycin	12152201	8
Caelo	Erythromycin	12152202	3
Caelo	Erythromycin	12152203	1
Caelo	Erythromycin	12152205	10
Caelo	Erythromycin	12152206	9
Caelo	Erythromycin	12152208	4
Caelo	Erythromycin	12156201	3
Caelo	Erythromycin	12156202	7
Caelo	Erythromycin	12156203	2
Caelo	Erythromycin	12156204	4
Caelo	Erythromycin	12156206	2
Caelo	Erythromycin	12156207	3
Caelo	Erythromycin	12156208	6
Caelo	Erythromycin	12E24-N04	1
Caelo	Erythromycin	13011810	1
Caelo	Erythromycin	1308016-01	2
Caelo	Erythromycin	1308016-02	1
Caelo	Erythromycin	13145504	1
Caelo	Erythromycin	1315501	1
Caelo	Erythromycin	13175501	6
Caelo	Erythromycin	13175502	4
Caelo	Erythromycin	13175503	8
Caelo	Erythromycin	13175504	6
Caelo	Erythromycin	13175504-3413310132	1
Caelo	Erythromycin	13175505	4
Caelo	Erythromycin	13175506	4
Caelo	Erythromycin	13175506-3559412014	1
Caelo	Erythromycin	13175601	10
Caelo	Erythromycin	131756017	1
Caelo	Erythromycin	13175603	11
Caelo	Erythromycin	13175604	7
Caelo	Erythromycin	13175607	8
Caelo	Erythromycin	13175608	6
Caelo	Erythromycin	13175610	1
Caelo	Erythromycin	13175611	5
Caelo	Erythromycin	13175612	2
Caelo	Erythromycin	13175801	10
Caelo	Erythromycin	13175802	8
Caelo	Erythromycin	13175803	8
Caelo	Erythromycin	13175804	2
Caelo	Erythromycin	13175808	2
Caelo	Erythromycin	13175809	5
Caelo	Erythromycin	13175810	4
Caelo	Erythromycin	13175811	8
Caelo	Erythromycin	13178756tzgklhj	1
Caelo	Erythromycin	13189001	8
Caelo	Erythromycin	13189002	7
Caelo	Erythromycin	13189004	5
Caelo	Erythromycin	13189006	3
Caelo	Erythromycin	13189007	2
Caelo	Erythromycin	132152108	1
Caelo	Erythromycin	13A02-N06	1
Caelo	Erythromycin	13D30-N01	3
Caelo	Erythromycin	13H22-N07	1
Caelo	Erythromycin	14/30-B01-300059	1
Caelo	Erythromycin	14/30-B01-308189	2
Caelo	Erythromycin	140044203	1
Caelo	Erythromycin	140440006	1
Caelo	Erythromycin	14044001	10

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Erythromycin	14044002	10
Caelo	Erythromycin	14044004	11
Caelo	Erythromycin	140440044	1
Caelo	Erythromycin	14044005	11
Caelo	Erythromycin	14044006	6
Caelo	Erythromycin	14044007	8
Caelo	Erythromycin	14044008	4
Caelo	Erythromycin	14044009	3
Caelo	Erythromycin	14044010	4
Caelo	Erythromycin	14044011	2
Caelo	Erythromycin	14044012	3
Caelo	Erythromycin	14044014	3
Caelo	Erythromycin	1404409	1
Caelo	Erythromycin	14044101	7
Caelo	Erythromycin	14044105	4
Caelo	Erythromycin	14044106	3
Caelo	Erythromycin	14044107	3
Caelo	Erythromycin	14044109	5
Caelo	Erythromycin	14044110	1
Caelo	Erythromycin	14044114	6
Caelo	Erythromycin	14044115	6
Caelo	Erythromycin	14044118	3
Caelo	Erythromycin	1404414	1
Caelo	Erythromycin	1404418	1
Caelo	Erythromycin	14044201	5
Caelo	Erythromycin	14044202	3
Caelo	Erythromycin	14044205	4
Caelo	Erythromycin	14044206	3
Caelo	Erythromycin	14044207	2
Caelo	Erythromycin	1409019	1
Caelo	Erythromycin	1409019-01	2
Caelo	Erythromycin	140901902	2
Caelo	Erythromycin	1409019-02	4
Caelo	Erythromycin	140930E	1
Caelo	Erythromycin	1414M-01362	1
Caelo	Erythromycin	1430b01300059	1
Caelo	Erythromycin	14B06-B35-290872	1
Caelo	Erythromycin	14B06-B35-290873	1
Caelo	Erythromycin	14b06-b35-293508	1
Caelo	Erythromycin	14F13-B02-296464	2
Caelo	Erythromycin	14F13-B02-300061	1
Caelo	Erythromycin	14I30-B01	1
Caelo	Erythromycin	14I30-B01-308789	1
Caelo	Erythromycin	150242813	1
Caelo	Erythromycin	15042601	2
Caelo	Erythromycin	15042602	8
Caelo	Erythromycin	15042603	6
Caelo	Erythromycin	15042604	3
Caelo	Erythromycin	15042605	9
Caelo	Erythromycin	15042606	1
Caelo	Erythromycin	15042608	3
Caelo	Erythromycin	15042609	8
Caelo	Erythromycin	15042610	10
Caelo	Erythromycin	15042611	5
Caelo	Erythromycin	15042611-20160504Ma1	1
Caelo	Erythromycin	15042612	7
Caelo	Erythromycin	15042613	4
Caelo	Erythromycin	15042701	12
Caelo	Erythromycin	15042702	4
Caelo	Erythromycin	15042703	9

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Erythromycin	15042704	9
Caelo	Erythromycin	15042705	12
Caelo	Erythromycin	15042706	10
Caelo	Erythromycin	15042707	1
Caelo	Erythromycin	15042711	14
Caelo	Erythromycin	150427704	1
Caelo	Erythromycin	150428	1
Caelo	Erythromycin	15042802	3
Caelo	Erythromycin	15042803	14
Caelo	Erythromycin	15042804	1
Caelo	Erythromycin	15042806	12
Caelo	Erythromycin	15042808	1
Caelo	Erythromycin	15042809	3
Caelo	Erythromycin	15042810	6
Caelo	Erythromycin	15042811	3
Caelo	Erythromycin	15042812	1
Caelo	Erythromycin	15042813	14
Caelo	Erythromycin	15042814	11
Caelo	Erythromycin	15042815	3
Caelo	Erythromycin	15042816	7
Caelo	Erythromycin	15042901	10
Caelo	Erythromycin	15042902	2
Caelo	Erythromycin	1504812	1
Caelo	Erythromycin	1504813	1
Caelo	Erythromycin	150803401	1
Caelo	Erythromycin	1508034-01	1
Caelo	Erythromycin	1508034-02	3
Caelo	Erythromycin	1524002	1
Caelo	Erythromycin	1524004	1
Caelo	Erythromycin	15245002	20
Caelo	Erythromycin	15245003	9
Caelo	Erythromycin	15245004	13
Caelo	Erythromycin	15245005	2
Caelo	Erythromycin	15245007	3
Caelo	Erythromycin	15245008	3
Caelo	Erythromycin	15245008I-041016-3	1
Caelo	Erythromycin	15245101	11
Caelo	Erythromycin	154042602	1
Caelo	Erythromycin	16/24-B10-341876	1
Caelo	Erythromycin	16017088303	1
Caelo	Erythromycin	1607038	1
Caelo	Erythromycin	160703801	2
Caelo	Erythromycin	1607038-01	4
Caelo	Erythromycin	1607038-02	10
Caelo	Erythromycin	16073038-02	1
Caelo	Erythromycin	160738-01	1
Caelo	Erythromycin	16076903	1
Caelo	Erythromycin	16079201	10
Caelo	Erythromycin	16079202	12
Caelo	Erythromycin	16079203	21
Caelo	Erythromycin	16079204	14
Caelo	Erythromycin	16079205	5
Caelo	Erythromycin	16079206	5
Caelo	Erythromycin	16079207	8
Caelo	Erythromycin	16079208	9
Caelo	Erythromycin	16079209	1
Caelo	Erythromycin	16079210	9
Caelo	Erythromycin	16079213	14
Caelo	Erythromycin	16079214	11
Caelo	Erythromycin	16079214-20170704Ma1	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Erythromycin	16079214-20171127Ma6	1
Caelo	Erythromycin	16079214-24417/1	1
Caelo	Erythromycin	16079216	8
Caelo	Erythromycin	16079501	20
Caelo	Erythromycin	16079502	15
Caelo	Erythromycin	16079503	8
Caelo	Erythromycin	16079505	3
Caelo	Erythromycin	16079506	7
Caelo	Erythromycin	16079507	1
Caelo	Erythromycin	16079509	29
Caelo	Erythromycin	16079510	9
Caelo	Erythromycin	16079511	10
Caelo	Erythromycin	16079512	5
Caelo	Erythromycin	16079513	11
Caelo	Erythromycin	16079514	1
Caelo	Erythromycin	16079515	1
Caelo	Erythromycin	160796	1
Caelo	Erythromycin	16079602	5
Caelo	Erythromycin	16079603	15
Caelo	Erythromycin	16079604	5
Caelo	Erythromycin	16079605	2
Caelo	Erythromycin	16079606	7
Caelo	Erythromycin	16079607	1
Caelo	Erythromycin	16079608	21
Caelo	Erythromycin	16079609	8
Caelo	Erythromycin	16079610	1
Caelo	Erythromycin	16079612	16
Caelo	Erythromycin	16079613	2
Caelo	Erythromycin	16079614	6
Caelo	Erythromycin	16079701	1
Caelo	Erythromycin	16079702	8
Caelo	Erythromycin	16079704	4
Caelo	Erythromycin	16091712	1
Caelo	Erythromycin	16979201	1
Caelo	Erythromycin	16G06-803	1
Caelo	Erythromycin	16G06-B03-324463	1
Caelo	Erythromycin	16G06-B03-324464	3
Caelo	Erythromycin	16G06-B03-324465	1
Caelo	Erythromycin	16G06-B03-324466	2
Caelo	Erythromycin	16G06B03329150	1
Caelo	Erythromycin	16G06-B03-329150	1
Caelo	Erythromycin	16i24-B10	1
Caelo	Erythromycin	16j24b1033673	1
Caelo	Erythromycin	16J24-B10-339487	1
Caelo	Erythromycin	16J24-B10-341875	1
Caelo	Erythromycin	16J24-B10-341876	1
Caelo	Erythromycin	16J24-B-341876	1
Caelo	Erythromycin	1705037-01	1
Caelo	Erythromycin	1705038	2
Caelo	Erythromycin	1705038_02	1
Caelo	Erythromycin	170503801	1
Caelo	Erythromycin	1705038-01	7
Caelo	Erythromycin	170503802	1
Caelo	Erythromycin	1705038-02	4
Caelo	Erythromycin	1705038-03	2
Caelo	Erythromycin	17068309	1
Caelo	Erythromycin	170718A	1
Caelo	Erythromycin	1708/8308	1
Caelo	Erythromycin	17086301	1
Caelo	Erythromycin	17088001	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Erythromycin	17088002	19
Caelo	Erythromycin	17088003	12
Caelo	Erythromycin	17088004	14
Caelo	Erythromycin	17088005	14
Caelo	Erythromycin	17088007	11
Caelo	Erythromycin	17088008	15
Caelo	Erythromycin	17088008-20180206Ma2	1
Caelo	Erythromycin	17088008-E20180112Ma	1
Caelo	Erythromycin	17088009	11
Caelo	Erythromycin	17088010	14
Caelo	Erythromycin	17088010-20180404Ma2	1
Caelo	Erythromycin	170880103	1
Caelo	Erythromycin	17088011	1
Caelo	Erythromycin	17088013	35
Caelo	Erythromycin	17088013/1250418	1
Caelo	Erythromycin	1708807	1
Caelo	Erythromycin	1708808	2
Caelo	Erythromycin	17088203	19
Caelo	Erythromycin	17088204	48
Caelo	Erythromycin	17088206	1
Caelo	Erythromycin	17088207	9
Caelo	Erythromycin	17088208	2
Caelo	Erythromycin	17088210	34
Caelo	Erythromycin	17088210-E20181115Ma	1
Caelo	Erythromycin	17088212	1
Caelo	Erythromycin	17088301	70
Caelo	Erythromycin	17088302	4
Caelo	Erythromycin	17088303	7
Caelo	Erythromycin	17088304	1
Caelo	Erythromycin	17088305	28
Caelo	Erythromycin	17088305031110172	1
Caelo	Erythromycin	17088306	38
Caelo	Erythromycin	17088308	12
Caelo	Erythromycin	17088309	22
Caelo	Erythromycin	17088401	8
Caelo	Erythromycin	17088402	17
Caelo	Erythromycin	17088403	25
Caelo	Erythromycin	17088403-20180619Ma1	1
Caelo	Erythromycin	17088403-E2081115Ma1	1
Caelo	Erythromycin	17088404	25
Caelo	Erythromycin	17088405	19
Caelo	Erythromycin	17088406	11
Caelo	Erythromycin	170888309	1
Caelo	Erythromycin	1709038-01	1
Caelo	Erythromycin	17219705	1
Caelo	Erythromycin	1780210	1
Caelo	Erythromycin	178824	1
Caelo	Erythromycin	1788402	1
Caelo	Erythromycin	180096302	1
Caelo	Erythromycin	18094606	1
Caelo	Erythromycin	18095303	1
Caelo	Erythromycin	1809604	1
Caelo	Erythromycin	180960405	1
Caelo	Erythromycin	18096201	25
Caelo	Erythromycin	180962011905013-04	1
Caelo	Erythromycin	18096202	14
Caelo	Erythromycin	18096203	1
Caelo	Erythromycin	18096204	5
Caelo	Erythromycin	18096205	26
Caelo	Erythromycin	18096206	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Erythromycin	18096207	2
Caelo	Erythromycin	18096208	17
Caelo	Erythromycin	18096209	29
Caelo	Erythromycin	18096210	12
Caelo	Erythromycin	18096211	10
Caelo	Erythromycin	1809630	1
Caelo	Erythromycin	18096302	19
Caelo	Erythromycin	18096303	15
Caelo	Erythromycin	18096304	5
Caelo	Erythromycin	18096305	3
Caelo	Erythromycin	180964001	27
Caelo	Erythromycin	180964002	7
Caelo	Erythromycin	180964003	15
Caelo	Erythromycin	180964004	4
Caelo	Erythromycin	180964005	4
Caelo	Erythromycin	18096401	33
Caelo	Erythromycin	18096403	13
Caelo	Erythromycin	18096404	9
Caelo	Erythromycin	18096405	24
Caelo	Erythromycin	18096406	30
Caelo	Erythromycin	180964403	1
Caelo	Erythromycin	1811019-01	6
Caelo	Erythromycin	1811019-02	1
Caelo	Erythromycin	18215001	3
Caelo	Erythromycin	18F05-B01-350907	1
Caelo	Erythromycin	18F05-B01-350908	1
Caelo	Erythromycin	18F05-B01-35096	1
Caelo	Erythromycin	18F05-B01-356705	1
Caelo	Erythromycin	18F05-B01-356706	2
Caelo	Erythromycin	18F05-B01-358087	1
Caelo	Erythromycin	19011908	1
Caelo	Erythromycin	1903060E	1
Caelo	Erythromycin	1906032-01	6
Caelo	Erythromycin	19071306	1
Caelo	Erythromycin	19096406	1
Caelo	Erythromycin	19C21B03361400	1
Caelo	Erythromycin	19L18-F02-367776	1
Caelo	Erythromycin	19L18-F02367779	1
Caelo	Erythromycin	200002258002	1
Caelo	Erythromycin	200002259007	1
Caelo	Erythromycin	200003731001	1
Caelo	Erythromycin	200003731004	1
Caelo	Erythromycin	200022259008	1
Caelo	Erythromycin	20002250002	1
Caelo	Erythromycin	20002258001	3
Caelo	Erythromycin	20002258002	20
Caelo	Erythromycin	20002258003	2
Caelo	Erythromycin	20002259002	24
Caelo	Erythromycin	20002259003	23
Caelo	Erythromycin	20002259003/4620	1
Caelo	Erythromycin	20002259004	4
Caelo	Erythromycin	20002259005	11
Caelo	Erythromycin	20002259006	26
Caelo	Erythromycin	20002259007	15
Caelo	Erythromycin	20002259008	2
Caelo	Erythromycin	20003431004	1
Caelo	Erythromycin	2000373007	1
Caelo	Erythromycin	2000373009	1
Caelo	Erythromycin	20003731001	23
Caelo	Erythromycin	20003731002	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Erythromycin	20003731003	25
Caelo	Erythromycin	20003731004	28
Caelo	Erythromycin	20003731005	27
Caelo	Erythromycin	20003732001	16
Caelo	Erythromycin	20003732002	7
Caelo	Erythromycin	20003732004	13
Caelo	Erythromycin	20003732005	6
Caelo	Erythromycin	20003732006	1
Caelo	Erythromycin	20003732007	11
Caelo	Erythromycin	20003732008	15
Caelo	Erythromycin	20003732009	28
Caelo	Erythromycin	20003732010	27
Caelo	Erythromycin	20003732011	3
Caelo	Erythromycin	20003733001	7
Caelo	Erythromycin	2000373731004	1
Caelo	Erythromycin	2000373732010	1
Caelo	Erythromycin	20003762010	1
Caelo	Erythromycin	20004278008	1
Caelo	Erythromycin	2002258002	1
Caelo	Erythromycin	2003731005	1
Caelo	Erythromycin	2003732011	1
Caelo	Erythromycin	2003733001	1
Caelo	Erythromycin	2007017-01	3
Caelo	Erythromycin	2010015-01	3
Caelo	Erythromycin	2010015-03	1
Caelo	Erythromycin	20122013D	1
Caelo	Erythromycin	20270912-3	1
Caelo	Erythromycin	20E18-F05-371567	1
Caelo	Erythromycin	20E18-F06	1
Caelo	Erythromycin	20E18-F06-372104	1
Caelo	Erythromycin	20I07-F06	1
Caelo	Erythromycin	2100100204	1
Caelo	Erythromycin	21002041001	8
Caelo	Erythromycin	21002041002	11
Caelo	Erythromycin	21002041003	3
Caelo	Erythromycin	21002041006	6
Caelo	Erythromycin	21002041007	13
Caelo	Erythromycin	21002041008	2
Caelo	Erythromycin	21002041009	4
Caelo	Erythromycin	21002041010	7
Caelo	Erythromycin	21002041012	1
Caelo	Erythromycin	21002041014	8
Caelo	Erythromycin	21002042001	15
Caelo	Erythromycin	21002044001	2
Caelo	Erythromycin	21002044002	3
Caelo	Erythromycin	210020441004	1
Caelo	Erythromycin	21002046001	3
Caelo	Erythromycin	21002053002	1
Caelo	Erythromycin	2100242001	1
Caelo	Erythromycin	21A26-F01	1
Caelo	Erythromycin	21A26-F01-376731	1
Caelo	Erythromycin	22001550001	3
Caelo	Erythromycin	22001550002	5
Caelo	Erythromycin	22002199001	1
Caelo	Erythromycin	22002200001	9
Caelo	Erythromycin	22002200002	4
Caelo	Erythromycin	22002200003	1
Caelo	Erythromycin	22002202001	1
Caelo	Erythromycin	22041302	1
Caelo	Erythromycin	23021710	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Erythromycin	24071402	1
Caelo	Erythromycin	24101312	1
Caelo	Erythromycin	26011402	1
Caelo	Erythromycin	27071202	1
Caelo	Erythromycin	2761	1
Caelo	Erythromycin	28041505	1
Caelo	Erythromycin	28101405	1
Caelo	Erythromycin	30011505	1
Caelo	Erythromycin	308160l	1
Caelo	Erythromycin	3092014B	1
Caelo	Erythromycin	3110195	1
Caelo	Erythromycin	3317	1
Caelo	Erythromycin	4316E-01362	1
Caelo	Erythromycin	5042604	1
Caelo	Erythromycin	5052015D	1
Caelo	Erythromycin	511111	1
Caelo	Erythromycin	59/AKD59	1
Caelo	Erythromycin	60/AKD4	1
Caelo	Erythromycin	618E-01362	1
Caelo	Erythromycin	80963021	1
Caelo	Erythromycin	Caelo	1
Caelo	Erythromycin	EB06/14	1
Caelo	Erythromycin	I31032016/1	1
Caeolo/Krieger	Erythromycin	17088004	1
Caeolo/Noweda	Erythromycin	13189007	1
Caeolo/Noweda	Erythromycin	16079603	1
Caesa / Alliance Hea...	Erythromycin	17088309	1
Caesar & Lorenz GmbH	Erythromycin	15042611	1
Caesar & Loretz GmbH...	Erythromycin	20003732009	1
Caesar & Loretz GmbH...	Erythromycin	20002259003	1
Caesar & Loretz GmbH...	Erythromycin	20003731005	1
Caesar & Loretz GmbH...	Erythromycin	18096211	1
Caesar & Loretz GmbH...	Erythromycin	18096401	1
Caesar & Loretz GmbH...	Erythromycin	18096405	2
Caesar & Loretz GmbH...	Erythromycin	18096406	1
Caesar & Loretz GmbH...	Erythromycin	17088404	1
Caesar & Loretz GmbH...	Erythromycin	18096201	1
Caesar & Loretz GmbH...	Erythromycin	18096208	1
Caesar & Loretz GmbH...	Erythromycin	18096406	1
Caesar & Loretz GmbH...	Erythromycin	22001550002	1
Caesar & Loretz GmbH...	Erythromycin	20003732002	1
Caesar & Loretz GmbH...	Erythromycin	180964005	1
Caesar & Loretz GmbH...	Erythromycin	18096401	1
Caesar & Loretz GmbH...	Erythromycin	10217208	1
Caesar & Loretz GmbH...	Erythromycin	13189002	1
Caesar & Loretz GmbH...	Erythromycin	17088003	1
Caesar & Loretz GmbH...	Erythromycin	20003731001	2
Caesar & Loretz GmbH...	Erythromycin	16079207	1
Caesar & Loretz GmbH...	Erythromycin	21002041002	1
Caesar & Loretz GmbH/ G	Erythromycin	18096201	1
Caesar & Loretz GmbH...	Erythromycin	20003732010	1
Caesar & Loretz GmbH/ GTH	Erythromycin	18096209	1
Caesar & Loretz GmbH...	Erythromycin	21002041010	1
Caesar & Loretz GmbH...	Erythromycin	20003731004	3
Caesar & Loretz GmbH...	Erythromycin	180964001	1
Caesar & Loretz GmbH...	Erythromycin	20003731004	1
Caesar & Loretz GmbH/AEP	Erythromycin	18096302	2
Caesar & Loretz GmbH/AEP	Erythromycin	22002200002	1
Caesar & Loretz GmbH/AHD	Erythromycin	20002259005	1
Caesar & Loretz GmbH/AHD	Erythromycin	20003733001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Erythromycin	17088303	1
Caesar & Loretz GmbH...	Erythromycin	20003731004	1
Caesar & Loretz GmbH...	Erythromycin	20003732008	1
Caesar & Loretz GmbH...	Erythromycin	20003732010	1
Caesar & Loretz GmbH...	Erythromycin	20002259006	2
Caesar & Loretz GmbH/E	Erythromycin	21002041001	1
Caesar & Loretz GmbH...	Erythromycin	18096404	1
Caesar & Loretz GmbH...	Erythromycin	20003732007	1
Caesar & Loretz GmbH/G	Erythromycin	20002258002	1
Caesar & Loretz GmbH/Gehe	Erythromycin	18096208	1
Caesar & Loretz GmbH/Gehe	Erythromycin	18096209	1
Caesar & Loretz GmbH/Gehe	Erythromycin	180964002	1
Caesar & Loretz GmbH/Gehe	Erythromycin	18096401	1
Caesar & Loretz GmbH/Gehe	Erythromycin	18096405	1
Caesar & Loretz GmbH/Gehe	Erythromycin	18096406	3
Caesar & Loretz GmbH/Gehe	Erythromycin	22002199001	1
Caesar & Loretz GmbH...	Erythromycin	20002258003	1
Caesar & Loretz GmbH...	Erythromycin	20003732002	1
Caesar & Loretz GmbH...	Erythromycin	21002041008	1
Caesar & Loretz GmbH...	Erythromycin	20002259002	1
Caesar & Loretz GmbH...	Erythromycin	20003731004	1
Caesar & Loretz GmbH...	Erythromycin	20003732010	1
Caesar & Loretz GmbH...	Erythromycin	21002041009	1
Caesar & Loretz GmbH...	Erythromycin	18096302	1
Caesar & Loretz GmbH...	Erythromycin	20002259002	1
Caesar & Loretz GmbH...	Erythromycin	20003731004	1
Caesar & Loretz GmbH...	Erythromycin	21002041001	1
Caesar & Loretz GmbH...	Erythromycin	21002042001	1
Caesar & Loretz GmbH/Kehr	Erythromycin	F05-3715605	1
Caesar & Loretz GmbH...	Erythromycin	20003731003	1
Caesar & Loretz GmbH...	Erythromycin	200201801	1
Caesar & Loretz GmbH...	Erythromycin	18096405	1
Caesar & Loretz GmbH...	Erythromycin	20002259007	1
Caesar & Loretz GmbH...	Erythromycin	20003731001	1
Caesar & Loretz GmbH...	Erythromycin	20003732008	1
Caesar & Loretz GmbH...	Erythromycin	21002041002	1
Caesar & Loretz GmbH/Ph	Erythromycin	1906032-01	1
Caesar & Loretz GmbH/Phoe	Erythromycin	20002258003	1
Caesar & Loretz GmbH...	Erythromycin	22002199001	1
Caesar & Loretz GmbH...	Erythromycin	180964003	2
Caesar & Loretz GmbH...	Erythromycin	20002259003	1
Caesar & Loretz GmbH...	Erythromycin	20002259005	1
Caesar & Loretz GmbH...	Erythromycin	20002259007	1
Caesar & Loretz GmbH...	Erythromycin	20003731005	1
Caesar & Loretz GmbH...	Erythromycin	20003732007	1
Caesar & Loretz GmbH...	Erythromycin	20003732008	1
Caesar & Loretz GmbH...	Erythromycin	20003732009	2
Caesar & Loretz GmbH...	Erythromycin	18096209	1
Caesar & Loretz GmbH...	Erythromycin	180964001	1
Caesar & Loretz GmbH...	Erythromycin	18096403	1
Caesar & Loretz GmbH...	Erythromycin	20002258002	1
Caesar & Loretz GmbH...	Erythromycin	20002259003	1
Caesar & Loretz GmbH...	Erythromycin	20003732008	1
Caesar & Loretz GmbH...	Erythromycin	20003732009	1
Caesar & Loretz GmbH...	Erythromycin	21002041002	2
Caesar & Loretz GmbH...	Erythromycin	21002041006	1
Caesar & Loretz GmbH...	Erythromycin	21002041007	2
Caesar & Loretz GmbH...	Erythromycin	21002042001	1
Caesar & Loretz GmbH...	Erythromycin	AP220827-07	1
Caesar & Loretz GmbH...	Erythromycin	21002044001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Wepa	Erythromycin	180964003	1
Caesar & Loretz GmbH	Erythromycin	15042814	1
Caesar & Loretz GmbH	Erythromycin	16079509	2
Caesar & Loretz GmbH	Erythromycin	17088005	1
Caesar & Loretz GmbH	Erythromycin	17088305	2
Caesar & Loretz GmbH	Erythromycin	17088306	6
Caesar & Loretz GmbH	Erythromycin	17088308	1
Caesar & Loretz GmbH	Erythromycin	17088309	8
Caesar & Loretz GmbH	Erythromycin	17088403	1
Caesar & Loretz GmbH	Erythromycin	17088404	2
Caesar & Loretz GmbH	Erythromycin	18096201	2
Caesar & Loretz GmbH	Erythromycin	18096203	1
Caesar & Loretz GmbH	Erythromycin	18096204	3
Caesar & Loretz GmbH	Erythromycin	18096205	5
Caesar & Loretz GmbH	Erythromycin	18096207	1
Caesar & Loretz GmbH	Erythromycin	18096208	3
Caesar & Loretz GmbH	Erythromycin	18096209	8
Caesar & Loretz GmbH	Erythromycin	18096210	6
Caesar & Loretz GmbH	Erythromycin	18096211	3
Caesar & Loretz GmbH	Erythromycin	18096302	2
Caesar & Loretz GmbH	Erythromycin	18096303	1
Caesar & Loretz GmbH	Erythromycin	18096304	1
Caesar & Loretz GmbH	Erythromycin	18096305	2
Caesar & Loretz GmbH	Erythromycin	180964001	2
Caesar & Loretz GmbH	Erythromycin	180964002	2
Caesar & Loretz GmbH	Erythromycin	180964003	8
Caesar & Loretz GmbH	Erythromycin	180964005	2
Caesar & Loretz GmbH	Erythromycin	18096401	18
Caesar & Loretz GmbH	Erythromycin	18096403	6
Caesar & Loretz GmbH	Erythromycin	18096404	1
Caesar & Loretz GmbH	Erythromycin	18096405	6
Caesar & Loretz GmbH	Erythromycin	18096406	6
Caesar & Loretz GmbH	Erythromycin	20002258002	1
Caesar & Loretz GmbH	Erythromycin	20002259002	4
Caesar & Loretz GmbH	Erythromycin	20002259003	7
Caesar & Loretz GmbH	Erythromycin	20002259005	4
Caesar & Loretz GmbH	Erythromycin	20002259006	8
CAESAR & LORETZ GMBH	Erythromycin	20002259006	2
Caesar & Loretz GmbH	Erythromycin	20002259007	4
Caesar & Loretz GmbH	Erythromycin	20002259008	1
Caesar & Loretz GmbH	Erythromycin	20003731001	10
Caesar & Loretz GmbH	Erythromycin	20003731002	1
Caesar & Loretz GmbH	Erythromycin	20003731003	6
Caesar & Loretz GmbH	Erythromycin	20003731004	6
Caesar & Loretz GmbH	Erythromycin	20003731005	10
Caesar & Loretz GmbH	Erythromycin	20003732001	3
Caesar & Loretz GmbH	Erythromycin	20003732002	1
Caesar & Loretz GmbH	Erythromycin	20003732004	2
Caesar & Loretz GmbH	Erythromycin	20003732007	9
Caesar & Loretz GmbH	Erythromycin	20003732008	17
Caesar & Loretz GmbH	Erythromycin	20003732009	7
Caesar & Loretz GmbH	Erythromycin	20003732010	14
Caesar & Loretz GmbH	Erythromycin	20003732011	1
Caesar & Loretz GmbH	Erythromycin	20003733001	8
Caesar & Loretz GmbH	Erythromycin	2002259005	2
Caesar & Loretz GmbH	Erythromycin	21002041002	8
Caesar & Loretz GmbH	Erythromycin	21002041003	4
Caesar & Loretz GmbH	Erythromycin	21002041004	5
Caesar & Loretz GmbH	Erythromycin	21002041008	1
Caesar & Loretz GmbH	Erythromycin	21002041009	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Erythromycin	21002041010	2
Caesar & Loretz GmbH	Erythromycin	21002041011	1
Caesar & Loretz GmbH	Erythromycin	21002041012	2
Caesar & Loretz GmbH	Erythromycin	21002041014	1
Caesar & Loretz GmbH	Erythromycin	21002042001	6
Caesar & Loretz GmbH	Erythromycin	21002044001	1
Caesar & Loretz GmbH	Erythromycin	21002046001	2
Caesar & Loretz GmbH	Erythromycin	22001550001	1
Caesar & Loretz GmbH	Erythromycin	22001550003	1
Caesar & Loretz GmbH	Erythromycin	22002200001	1
Caesar & Loretz GmbH	Erythromycin	2206001-01	1
Caesar & Loretz GmbH	Erythromycin	F02-3677709	3
Caesar & Loretz Hild...	Erythromycin	180964001	1
Caesar & Loretz Hilden	Erythromycin	17088305	1
Caesar & Loretz Hilden	Erythromycin	18096208	1
Caesar & Loretz/AHC	Erythromycin	15042813	1
Caesar & Loretz/AHD	Erythromycin	20002258002	1
Caesar & Loretz/Phönix	Erythromycin	20003732004	1
Caesar & Loretz/Sanacorp	Erythromycin	18096201	2
Caesar / Gehe	Erythromycin	15042705	1
Caesar / Gehe	Erythromycin	17088402	1
Caesar u. Loretz/Noweda	Erythromycin	16079209	1
Caesar und Loretz	Erythromycin	17088210	1
Caesar& Loretz GmbH	Erythromycin	17088305	1
Caesar&Lorenz/AHD	Erythromycin	18096303	1
Caesar&Loretz GmbH /Anzag	Erythromycin	15042610	1
Caesar&Loretz GmbH	Erythromycin	15042807	1
Caesar&Loretz GmbH	Erythromycin	20002259001	1
Caesar&Loretz GmbH	Erythromycin	21002044002	1
Caesar&loretz,Phoenix	Erythromycin	13175602	1
Caesar&loretz,Phoenix	Erythromycin	14044004	1
caesar&loretz,phönix	Erythromycin	15042603	1
Caesar/Loretz/Noweda	Erythromycin	15042610	1
Calo/AHD	Erythromycin	15042605	1
Cealo / Noweda	Erythromycin	1205036-02	1
Cealo/ Anzag	Erythromycin	16079603	2
Cealo/ Phoenix	Erythromycin	17088210	1
Cealo/Alliance Healthcare	Erythromycin	17088309	1
Cealo/Sanacorp	Erythromycin	180964003	1
Cealo	Erythromycin	16079513	1
Celo/Kehr	Erythromycin	16079608	1
Ebert & Jacobi	Erythromycin	15042611	1
Ebert & Jacobi	Erythromycin	15245007	1
Eigenherstellung	Erythromycin	14044006	1
EuRho / 2	Erythromycin	1811019-01	2
EuRho / Alliance	Erythromycin	2007017-01	1
EuRho / Noweda	Erythromycin	700770	1
EuRho 08.08.2013Alli...	Erythromycin	1205036-01	1
EuRho/ AHD	Erythromycin	1705038-01	1
EuRho/ Anzag	Erythromycin	211124(2010014-01)	1
EuRho/ NOWEDA	Erythromycin	1906032-01	1
EuRho/ Noweda	Erythromycin	2010015-02	1
EuRho/Gehe	Erythromycin	1409019-01	1
EuRho/Gehe	Erythromycin	1811019-01	1
EuRho/Gehe	Erythromycin	1906032-01	1
EuRho/Gehe	Erythromycin	2010014-01	1
EuRho/Noweda	Erythromycin	1508034-02	1
EuRho/Noweda	Erythromycin	1705038-01	1
EuRho/Noweda	Erythromycin	2002018-01	1
EuRho/Noweda	Erythromycin	2206001-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho/Phoenix	Erythromycin	2206001-01	2
EuRho/Phönix	Erythromycin	1106036-05	1
EuRho/Phönix	Erythromycin	1205035	1
EuRho/Phönix	Erythromycin	1308016-02	1
EuRho/Phönix	Erythromycin	1811019-01	1
EuRho/Phönix	Erythromycin	2002018-01	1
Eurho/Phönix	Erythromycin	2010014-02	1
EuRho/Sanacorp	Erythromycin	2010014-01	1
EuRho/Sanacorp	Erythromycin	2301053-01	1
EuRho	Erythromycin	1205035-01	1
EuRho	Erythromycin	1205035-02	1
EuRho	Erythromycin	1205036-01	1
EuRho	Erythromycin	1308016-02	3
EuRho	Erythromycin	1705038-01	1
EuRho	Erythromycin	1705038-02	1
EuRho	Erythromycin	1705038-03	1
EuRho	Erythromycin	1811019-01	2
EuRho	Erythromycin	1906032-01	1
EuRho	Erythromycin	2002018-01	1
EuRho	Erythromycin	2007017-01	2
EuRho	Erythromycin	2010014-02	1
Eurho	Erythromycin	2010015-01	1
EuRho	Erythromycin	2010015-01	1
EuRho	Erythromycin	2010015-03	2
Euro CT Phönix	Erythromycin	13175604	1
Euro OCT / Krieger	Erythromycin	2007017-01	1
Euro OCT / Krieger	Erythromycin	2010014-01	1
Euro Oct/Phoenix	Erythromycin	1705038-03	1
EURO OGT / Anzag	Erythromycin	1409019-01	1
Euro OT	Erythromycin	1409019-02	1
Euro OTC	Erythromycin	100(2002018-01)	1
Euro OTC	Erythromycin	101(2007017-01)	1
Euro OTC	Erythromycin	1013u-01362	1
Euro OTC	Erythromycin	1106036-04	1
Euro OTC	Erythromycin	1106036-05	6
Euro OTC	Erythromycin	111811019-02	1
Euro OTC	Erythromycin	1205035-01	13
Euro OTC	Erythromycin	120503502	1
Euro OTC	Erythromycin	1205035-02	17
Euro OTC	Erythromycin	1205036/02	1
Euro OTC	Erythromycin	120503601	1
Euro OTC	Erythromycin	1205036-01	7
Euro OTC	Erythromycin	120503602	2
Euro OTC	Erythromycin	1205036-02	9
Euro OTC	Erythromycin	12A02-N06	1
Euro OTC	Erythromycin	130801601	6
Euro OTC	Erythromycin	1308016-01	28
Euro OTC	Erythromycin	130801602	2
Euro OTC	Erythromycin	1308016-02	26
Euro OTC	Erythromycin	13175505	1
Euro OTC	Erythromycin	14044205	1
Euro OTC	Erythromycin	140901901	3
Euro OTC	Erythromycin	1409019-01	30
Euro OTC	Erythromycin	1409019-01Mg100g	1
Euro OTC	Erythromycin	140901902	1
Euro OTC	Erythromycin	1409019-02	53
Euro OTC	Erythromycin	1409019-02Gehe	1
Euro OTC	Erythromycin	14090-9-01	1
Euro OTC	Erythromycin	140919-02	2
Euro OTC	Erythromycin	15042810	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Erythromycin	15080-01	1
Euro OTC	Erythromycin	1508034	1
Euro OTC	Erythromycin	150803401	1
Euro OTC	Erythromycin	1508034-01	37
Euro OTC	Erythromycin	1508034-02	18
Euro OTC	Erythromycin	1508034-02Mg100g	1
Euro OTC	Erythromycin	150834-01	1
Euro OTC	Erythromycin	15245002	1
Euro OTC	Erythromycin	15245008	1
Euro OTC	Erythromycin	15245101	1
Euro OTC	Erythromycin	1607038	2
Euro OTC	Erythromycin	1607038/01	1
Euro OTC	Erythromycin	160703801	5
Euro OTC	Erythromycin	1607038-01	81
Euro OTC	Erythromycin	160703802	2
Euro OTC	Erythromycin	1607038-02	91
Euro OTC	Erythromycin	1607038-2	1
Euro OTC	Erythromycin	16079206	1
Euro OTC	Erythromycin	167038-01	1
Euro OTC	Erythromycin	167038-02	1
Euro OTC	Erythromycin	16G06-B03-329150	1
Euro OTC	Erythromycin	170503038-03	1
Euro OTC	Erythromycin	1705037-01	1
Euro OTC	Erythromycin	1705038	3
Euro OTC	Erythromycin	1705038_01	1
Euro OTC	Erythromycin	170503801	2
Euro OTC	Erythromycin	1705038-01	143
Euro OTC	Erythromycin	170503802	1
Euro OTC	Erythromycin	1705038-02	37
Euro OTC	Erythromycin	170503803	2
Euro OTC	Erythromycin	1705038-03	54
Euro OTC	Erythromycin	1705038-04	1
Euro OTC	Erythromycin	1705039-01	1
Euro OTC	Erythromycin	170538-03	1
Euro OTC	Erythromycin	17088005	1
Euro OTC	Erythromycin	17088203	2
Euro OTC	Erythromycin	17088204	2
Euro OTC	Erythromycin	17088210	4
Euro OTC	Erythromycin	180201E/1705038-01	1
Euro OTC	Erythromycin	181019-01	1
Euro OTC	Erythromycin	18110019-01	1
Euro OTC	Erythromycin	1811019_02	1
Euro OTC	Erythromycin	1811019-01	92
Euro OTC	Erythromycin	181101902	1
Euro OTC	Erythromycin	1811019-02	13
Euro OTC	Erythromycin	1811019-2	1
Euro OTC	Erythromycin	18111019	1
Euro OTC	Erythromycin	181119-01	1
Euro OTC	Erythromycin	19006032-01	1
Euro OTC	Erythromycin	1906032	3
Euro OTC	Erythromycin	190603201	7
Euro OTC	Erythromycin	1906032-01	106
Euro OTC	Erythromycin	1906032-02	19
Euro OTC	Erythromycin	1906032-03	3
Euro OTC	Erythromycin	190603301	1
Euro OTC	Erythromycin	190632-01	1
Euro OTC	Erythromycin	200201801	2
Euro OTC	Erythromycin	2002018-01	102
Euro OTC	Erythromycin	2002018-1	1
Euro OTC	Erythromycin	2002038-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Erythromycin	20022018-01	2
Euro OTC	Erythromycin	2007017	1
Euro OTC	Erythromycin	20070170-01	1
Euro OTC	Erythromycin	200701701	4
Euro OTC	Erythromycin	2007017-01	100
Euro OTC	Erythromycin	2007017-04	1
Euro OTC	Erythromycin	20100014-01	1
Euro OTC	Erythromycin	2010012-01	1
Euro OTC	Erythromycin	201001401	3
Euro OTC	Erythromycin	2010014-01	77
Euro OTC	Erythromycin	2010014-02	27
Euro OTC	Erythromycin	201001501	1
Euro OTC	Erythromycin	2010015-01	55
Euro OTC	Erythromycin	2010015-02	13
Euro OTC	Erythromycin	201001503	1
Euro OTC	Erythromycin	2010015-03	20
Euro OTC	Erythromycin	201004-01	1
Euro OTC	Erythromycin	21A26-F01-376732	2
Euro OTC	Erythromycin	2206001-01	23
Euro OTC	Erythromycin	220712(2010014-02)	1
Euro OTC	Erythromycin	2301053-01	5
Euro OTC	Erythromycin	2301053-02	3
Euro OTC	Erythromycin	31K190P	1
Euro OTC	Erythromycin	3613A1362	1
Euro OTC	Erythromycin	4112Q-01362	1
Euro OTC	Erythromycin	4914659	1
Euro OTC	Erythromycin	700770	1
Euro OTC	Erythromycin	80616-4	1
Euro OTC	Erythromycin	95(1705038-02	1
Euro OTC	Erythromycin	96(1811019-01)	1
Euro OTC	Erythromycin	97(1811019-02)	1
Euro OTC	Erythromycin	CEPEB022C22P	1
Euro OTC	Erythromycin	EBC/20-016	1
Euro OTC	Erythromycin	EBS/1205-M-040	1
Euro OTC	Erythromycin	EBS/1307-BM-001	1
Euro OTC	Erythromycin	EBS/1701-BM-001	4
Euro OTC	Erythromycin	EBS/18-M-003	1
Euro OTC	Erythromycin	EBS/19-022	5
Euro OTC	Erythromycin	EBS/20-016	1
Euro OTC	Erythromycin	EBS/20-040	1
Euro OTC	Erythromycin	EBS/20-041	1
Euro OTC	Erythromycin	EBS18M003	1
Euro OTC	Erythromycin	EM04022021	1
Euro OTC	Erythromycin	F02-3687508	1
Euro/ANZAG	Erythromycin	1705038-03	1
Euro/Gehe	Erythromycin	1508034-01	1
Euro/Gehe	Erythromycin	1607038-02	1
Euro/Gehe	Erythromycin	1705038-01	2
Euro/Krieger	Erythromycin	1607038-01	1
Euro/Krieger	Erythromycin	1906032-01	2
Euro/Noweda	Erythromycin	1811019-01	2
Euro/Phönix	Erythromycin	1705038-02	1
Euro/Phönix	Erythromycin	1811019-01	1
Euro/Phönix	Erythromycin	2007017-01	1
Euro/Sanacorp	Erythromycin	1607038-02	1
Euro/Sanacorp	Erythromycin	1705038-01	1
Euro	Erythromycin	1308016-02	1
euroct/gehe	Erythromycin	1308016-01	1
euroct/gehe	Erythromycin	1308016-02	2
Euroct/Gehe	Erythromycin	1409019-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Europharm/Otto	Erythromycin	1106036-05	2
EuroTOC / Noweda	Erythromycin	1409019-02	1
EurPS	Erythromycin	1409019-02	3
fagr	Erythromycin	13A02-N06	1
Fagron	Erythromycin		6
Fagron	Erythromycin	114-07-8	1
Fagron	Erythromycin	11D13-N09	2
Fagron	Erythromycin	11J06-N05	2
Fagron	Erythromycin	11J06-No5	1
Fagron	Erythromycin	1205036-01	1
Fagron	Erythromycin	12E24-N04	14
Fagron	Erythromycin	12E24-No4	1
Fagron	Erythromycin	12J30-N01	13
Fagron	Erythromycin	13175503	1
Fagron	Erythromycin	13175602	1
Fagron	Erythromycin	13175608	1
Fagron	Erythromycin	13175803	1
Fagron	Erythromycin	13175810	1
Fagron	Erythromycin	13A02N06	1
Fagron	Erythromycin	13A02-N06	9
Fagron	Erythromycin	13A02-N-06	1
Fagron	Erythromycin	13A02-N060571/680	1
Fagron	Erythromycin	13A02-No6	1
Fagron	Erythromycin	13d30-n01	1
Fagron	Erythromycin	13D30N01	1
Fagron	Erythromycin	13D30-N01	23
Fagron	Erythromycin	13D30-N01003/456	1
Fagron	Erythromycin	13D30-N010278/730	1
Fagron	Erythromycin	13D30-N010336/730	1
Fagron	Erythromycin	13f12-n21	1
Fagron	Erythromycin	13F12-N21	24
Fagron	Erythromycin	13H22-N07	7
Fagron	Erythromycin	13H22-N070126/246	1
Fagron	Erythromycin	13H22-N070228/246	1
Fagron	Erythromycin	14/30-B01	1
Fagron	Erythromycin	14/30-B01_308790	1
Fagron	Erythromycin	14/30B01300060	1
Fagron	Erythromycin	14/30-B01-300060	3
Fagron	Erythromycin	14/30B0130050	1
Fagron	Erythromycin	14/30-B01-303884	1
Fagron	Erythromycin	14/30-B01-308189	2
Fagron	Erythromycin	14/30-B01-308789	3
Fagron	Erythromycin	1409019-02	5
Fagron	Erythromycin	1430B01300059	1
Fagron	Erythromycin	1430-b01-300060	1
Fagron	Erythromycin	1430B01303884	1
Fagron	Erythromycin	1430-B01-303884	1
Fagron	Erythromycin	1430-B01-308789	1
Fagron	Erythromycin	14806-B35-290874	1
Fagron	Erythromycin	14B06-35-290873	1
Fagron	Erythromycin	14B06-B35	11
Fagron	Erythromycin	14B06-B35-290866	4
Fagron	Erythromycin	14b06-b35-290872	1
Fagron	Erythromycin	14B06-B35-290872	5
Fagron	Erythromycin	14B06-B35290873	1
Fagron	Erythromycin	14B06-B35-290873	4
Fagron	Erythromycin	14B06-B35-290874	3
Fagron	Erythromycin	14B06-B35-290875	8
Fagron	Erythromycin	14B06-B35-293508	2
Fagron	Erythromycin	14b06-b35-293509	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Erythromycin	14B06-B35-293509	7
Fagron	Erythromycin	14b06b5293508	1
Fagron	Erythromycin	14F13-B02	2
Fagron	Erythromycin	14F13-B02-293487	1
Fagron	Erythromycin	14F13-B02-293488	3
Fagron	Erythromycin	14F13-B02-293490	2
Fagron	Erythromycin	14F13-B02-293511	3
Fagron	Erythromycin	14F13-B02-296464	3
Fagron	Erythromycin	14F13-B02-300061	3
Fagron	Erythromycin	14F13-B12-300061	1
Fagron	Erythromycin	14I30B01	1
Fagron	Erythromycin	14I30-B01	5
Fagron	Erythromycin	14I30-B01-3000060	1
Fagron	Erythromycin	14I30-B01-300050	2
Fagron	Erythromycin	14i30b01-300059	1
Fagron	Erythromycin	14I30-B01-300060	2
Fagron	Erythromycin	14I30-B01-300062	3
Fagron	Erythromycin	14I30-B01-300063	1
Fagron	Erythromycin	14i30-b01-303884	1
Fagron	Erythromycin	14I30-B01-303884	7
Fagron	Erythromycin	14I30-B01-306927	3
Fagron	Erythromycin	14I30-B01-308188	4
Fagron	Erythromycin	14I30B01308189	1
Fagron	Erythromycin	14I30-B01-308189	1
Fagron	Erythromycin	14I30-B01-308789	1
Fagron	Erythromycin	14i30-b01-311166	1
Fagron	Erythromycin	14I30-B01-311166	2
Fagron	Erythromycin	1508034-01	2
Fagron	Erythromycin	16/24-B10-329158	1
Fagron	Erythromycin	16/24-B10-339487	2
Fagron	Erythromycin	16/24-B10-341875	1
Fagron	Erythromycin	16/24-B10-341876	1
Fagron	Erythromycin	16079208	1
Fagron	Erythromycin	16079608	1
Fagron	Erythromycin	16G06_B03_324466	1
Fagron	Erythromycin	16G06-B03	11
Fagron	Erythromycin	16G06-B03_0003	1
Fagron	Erythromycin	16G06-B03-324462	3
Fagron	Erythromycin	16g06-b03-324463	2
Fagron	Erythromycin	16G06-B03-324463	12
Fagron	Erythromycin	16G06-B03324464	1
Fagron	Erythromycin	16G06-B03-324464	13
Fagron	Erythromycin	16G06-B03-324465	7
Fagron	Erythromycin	16G06-B03-324466	7
Fagron	Erythromycin	16G06B03-329149	1
Fagron	Erythromycin	16G06-B03-329149	4
Fagron	Erythromycin	16g06-b03-329150	1
Fagron	Erythromycin	16G06-B03-329150	6
Fagron	Erythromycin	16G06-B03-329152	2
Fagron	Erythromycin	16G06-B03-329157	6
Fagron	Erythromycin	16G06-B03-324463	1
Fagron	Erythromycin	16G08-B03	1
Fagron	Erythromycin	16J24_B10_339487	1
Fagron	Erythromycin	16j24-b10	1
Fagron	Erythromycin	16J24-B10	8
Fagron	Erythromycin	16J24-B10-329154	3
Fagron	Erythromycin	16j24-b10-329155	1
Fagron	Erythromycin	16J24-b10-329155	1
Fagron	Erythromycin	16J24-B10-329155	4
Fagron	Erythromycin	16J24-B10-329156	10

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Erythromycin	16j24-b10-329158	1
Fagron	Erythromycin	16J24-B10-329158	3
Fagron	Erythromycin	16J24-B10-336735	7
Fagron	Erythromycin	16j24-b10-336736	1
Fagron	Erythromycin	16J24-B10-336736	4
Fagron	Erythromycin	16J24-B10-3367363	1
Fagron	Erythromycin	16J24-B10338558	1
Fagron	Erythromycin	16J24-B10-338558	1
Fagron	Erythromycin	16J24-B10-338559	1
Fagron	Erythromycin	16j24-b10-339487	1
Fagron	Erythromycin	16J24-B10-339487	9
Fagron	Erythromycin	16J24-B10-339488	3
Fagron	Erythromycin	16J24-B10-341875	7
Fagron	Erythromycin	16J24-B10-341876	1
Fagron	Erythromycin	16J24-B10-341877	1
Fagron	Erythromycin	16-j24-B10-346206	1
Fagron	Erythromycin	16J24-B10-346206	4
Fagron	Erythromycin	16J24-B10-358088	1
Fagron	Erythromycin	16J25-B10-329155	1
Fagron	Erythromycin	1705038-01	3
Fagron	Erythromycin	17088005	1
Fagron	Erythromycin	17088211	1
Fagron	Erythromycin	17088402	1
Fagron	Erythromycin	18096205	1
Fagron	Erythromycin	18096208	2
Fagron	Erythromycin	1811019-01	1
Fagron	Erythromycin	18f01-b0a-353587	1
Fagron	Erythromycin	18F05	1
Fagron	Erythromycin	18F058-B01-352501	1
Fagron	Erythromycin	18f05-b01	1
Fagron	Erythromycin	18F05-B01	7
Fagron	Erythromycin	18F-05-B01	1
Fagron	Erythromycin	18F05-B01-350897	1
Fagron	Erythromycin	18F05-B01-350906	11
Fagron	Erythromycin	18F05-B01-350907	5
Fagron	Erythromycin	18f05-b01-350908	1
Fagron	Erythromycin	18F05-B01-350908	12
Fagron	Erythromycin	18F05-B01-350909	2
Fagron	Erythromycin	18F05-B01-352500	7
Fagron	Erythromycin	18f05-b01-352501	1
Fagron	Erythromycin	18F05-B01-352501	3
Fagron	Erythromycin	18F05-B01-35358	1
Fagron	Erythromycin	18f05-b01-353586	1
Fagron	Erythromycin	18F05-B01-353586	8
Fagron	Erythromycin	18F05-B01-353587	8
Fagron	Erythromycin	18F05-B01-353588	3
Fagron	Erythromycin	18F05-B01-35387	1
Fagron	Erythromycin	18F05-B01-354817	2
Fagron	Erythromycin	18F05-B01-354818	1
Fagron	Erythromycin	18F05-B01-355773	1
Fagron	Erythromycin	18F05-B01-356076	1
Fagron	Erythromycin	18f05-b01-356705	1
Fagron	Erythromycin	18F05-B01-356705	5
Fagron	Erythromycin	18F05-B01-356706	2
Fagron	Erythromycin	18F05-B01-356707	8
Fagron	Erythromycin	18f05-b01-358087	1
Fagron	Erythromycin	18F05-B01-358087	4
Fagron	Erythromycin	18F05-B01-358088	7
Fagron	Erythromycin	18F05-B01-358362	1
Fagron	Erythromycin	18F05-B01-3586707	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Erythromycin	18F05-b01-359011	1
Fagron	Erythromycin	18F05-B01-359011	1
Fagron	Erythromycin	19C21	1
Fagron	Erythromycin	19C21_B03_361400	1
Fagron	Erythromycin	19C21_B03_361402	1
Fagron	Erythromycin	19C21_B03B19	1
Fagron	Erythromycin	19c21b03	1
Fagron	Erythromycin	19C21-B03	11
Fagron	Erythromycin	19C21-B03-0003	1
Fagron	Erythromycin	19c21b03361400	1
Fagron	Erythromycin	19C21-B03-361400	13
Fagron	Erythromycin	19c21b03361401	1
Fagron	Erythromycin	19C21-B03-361401	9
Fagron	Erythromycin	19C21-B03-361402	12
Fagron	Erythromycin	19c21b03361724	1
Fagron	Erythromycin	19C21B03361724	2
Fagron	Erythromycin	19C21-B03-361724	15
Fagron	Erythromycin	19C21-B03361725	1
Fagron	Erythromycin	19C21-B03-361725	12
Fagron	Erythromycin	19C21-B03-361726	3
Fagron	Erythromycin	19C21-B03-361726	1
Fagron	Erythromycin	19L18/F02/367780	1
Fagron	Erythromycin	19L18-F02	9
Fagron	Erythromycin	19L-18F02	1
Fagron	Erythromycin	19L18-F02-3677	1
Fagron	Erythromycin	19L18-F02-36776	1
Fagron	Erythromycin	19L18-F02-367776	1
Fagron	Erythromycin	19L18-F02-367777	9
Fagron	Erythromycin	19L18F02367778	1
Fagron	Erythromycin	19L18-F02-367778	11
Fagron	Erythromycin	19L18-F02-367779	12
Fagron	Erythromycin	19L18-F02-36778	2
Fagron	Erythromycin	19L18F02367780	1
Fagron	Erythromycin	19L18-F02-367780	2
Fagron	Erythromycin	19L18-F02-3677803	1
Fagron	Erythromycin	19L18-F02-367783	1
Fagron	Erythromycin	19L18-F02-367784	4
Fagron	Erythromycin	19L18-F02-368758	6
Fagron	Erythromycin	19L18-F02P-200319-4	1
Fagron	Erythromycin	19L18-FO2	1
Fagron	Erythromycin	19L18-FO2-367776	1
Fagron	Erythromycin	19L18-FO2-367778	1
Fagron	Erythromycin	19L18-Fo2-367779	1
Fagron	Erythromycin	19L18-FO2-367779	3
Fagron	Erythromycin	19L18-FO2-367784	2
Fagron	Erythromycin	19L18-FO2-368758	1
Fagron	Erythromycin	20/07-F06-375516	3
Fagron	Erythromycin	20107-F06	1
Fagron	Erythromycin	20107F06373880	1
Fagron	Erythromycin	20107-F06-373880	1
Fagron	Erythromycin	20107-F06375516	1
Fagron	Erythromycin	20107-F06-375516	4
Fagron	Erythromycin	20E18-F01-371571	1
Fagron	Erythromycin	20E18-F05	1
Fagron	Erythromycin	20E18-F05-371563	6
Fagron	Erythromycin	20E18-F05-371564	4
Fagron	Erythromycin	20E18-F05371565	3
Fagron	Erythromycin	20E18-F05-371565	5
Fagron	Erythromycin	20E18-F05-371566	4
Fagron	Erythromycin	20E18-F05-371567	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Erythromycin	20E18-F06	9
Fagron	Erythromycin	20E18-F06-371204	1
Fagron	Erythromycin	20E18F06371570	1
Fagron	Erythromycin	20E18-F06371570	1
Fagron	Erythromycin	20E18-F06-371570	2
Fagron	Erythromycin	20E18-F06371571	1
Fagron	Erythromycin	20E18-F06-371571	7
Fagron	Erythromycin	20e18-F06-371572	1
Fagron	Erythromycin	20E18-F06-371572	2
Fagron	Erythromycin	20E18F06371573	1
Fagron	Erythromycin	20E18-F06-371573	7
Fagron	Erythromycin	20E18-F06-371573	1
Fagron	Erythromycin	20E18-F06-372103	10
Fagron	Erythromycin	20E18-F06-372104	30
Fagron	Erythromycin	20E18-F06	1
Fagron	Erythromycin	20I07-F06-373880	3
Fagron	Erythromycin	20I07-F06-3755106	1
Fagron	Erythromycin	20I07-f06-375516	1
Fagron	Erythromycin	20I07-F06-375516	8
Fagron	Erythromycin	20I07-F06-375516	1
Fagron	Erythromycin	20I17-F06-375516	1
Fagron	Erythromycin	20l07-F06-375516	1
Fagron	Erythromycin	21/13-B02	1
Fagron	Erythromycin	21/13-B02-213864	2
Fagron	Erythromycin	21/13-B02-213865	1
Fagron	Erythromycin	21/13-BO2-213864	1
Fagron	Erythromycin	21113-B02-213864	1
Fagron	Erythromycin	21113b02213865	1
Fagron	Erythromycin	21A26-F01	3
Fagron	Erythromycin	21A26-F01-37631	1
Fagron	Erythromycin	21A26-F01-376730	8
Fagron	Erythromycin	21A26-F01376731	2
Fagron	Erythromycin	21A26-F01-376731	18
Fagron	Erythromycin	21a26-f01-376732	1
Fagron	Erythromycin	21A26-F01-376732	15
Fagron	Erythromycin	21A26-F01-376734	5
Fagron	Erythromycin	21A26-Fo1-376731	2
Fagron	Erythromycin	21A26-FO1-376732	1
Fagron	Erythromycin	21F02-F02-379295	6
Fagron	Erythromycin	21I13-B02-213770	2
Fagron	Erythromycin	21I13-B02-213864	3
Fagron	Erythromycin	21I13-B02-213865	6
Fagron	Erythromycin	21113-B02-213864	1
Fagron	Erythromycin	21113-BO2-213864	1
Fagron	Erythromycin	21113-BO2-213865	1
Fagron	Erythromycin	220401E	1
Fagron	Erythromycin	22102001	1
Fagron	Erythromycin	23D27-Bo1-227928	1
Fagron	Erythromycin	20E18-F06-372104	1
Fagron	Erythromycin	3000-50	1
Fagron	Erythromycin	300059	1
Fagron	Erythromycin	31K1900P	1
Fagron	Erythromycin	3D2000P	1
Fagron	Erythromycin	4212E-01362	1
Fagron	Erythromycin	4H21P	1
Fagron	Erythromycin	510211362	1
Fagron	Erythromycin	700770-0002	1
Fagron	Erythromycin	700770-0007P-190312	1
Fagron	Erythromycin	B01-3590101	1
Fagron	Erythromycin	B02-2138604	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Erythromycin	B02-213864	1
Fagron	Erythromycin	BO2-2138604	1
Fagron	Erythromycin	CEFEB001E18	1
Fagron	Erythromycin	cepb001e18	1
Fagron	Erythromycin	CEPEB001E18	2
Fagron	Erythromycin	CEPEB003D20P	4
Fagron	Erythromycin	CEPEB004H21P	2
Fagron	Erythromycin	CEPEB032B19	1
Fagron	Erythromycin	cepeb039g20p	1
Fagron	Erythromycin	CEPEB039G20P	1
Fagron	Erythromycin	CEPEB084A21	1
Fagron	Erythromycin	E-030613-1	1
Fagron	Erythromycin	E18F06-372104	1
Fagron	Erythromycin	E-250213-2	1
Fagron	Erythromycin	EB022E14	2
Fagron	Erythromycin	EB032J13	4
Fagron	Erythromycin	EB068/14	1
Fagron	Erythromycin	EB06814	1
Fagron	Erythromycin	EB078B13	1
Fagron	Erythromycin	EBS/1201-008	2
Fagron	Erythromycin	f02-3677707	1
Fagron	Erythromycin	F02-3677709	2
Fagron	Erythromycin	F02-3677803	1
Fagron	Erythromycin	F02-3677804	6
Fagron	Erythromycin	F05-3715606	1
Fagron	Erythromycin	F06-3715700	3
Fagron	Erythromycin	F06-3715703	2
Fagron	Erythromycin	F06-3721004	4
Fagron	Erythromycin	F06-3738800	1
Fagron	Erythromycin	F06-3755106	4
Fagron	Erythromycin	FO6-3715701	1
Fagron	Erythromycin	OEBA/0010516	2
Fagron	Erythromycin	OEBA/0020516	2
Fagron	Erythromycin	P-26041922/356705	1
Fargon/GEHE	Erythromycin	19C21-B03	1
Fargon/Gehe	Erythromycin	19C21-B03-361725	1
Fargon/GEHE	Erythromycin	19C21-B03-361725	1
Fargon/Noweda	Erythromycin	18F05-B01-356705	1
Fargon/Phoenix	Erythromycin	18F05-B01-358088	2
Fargon/Sanacorp	Erythromycin	16J24-B10-329158	1
Fargon	Erythromycin	19c21-b03-361725	1
Fargon	Erythromycin	20E18-F05-371566	1
Fargron / Gehe	Erythromycin	18F05-B01-350907	1
Fiebig	Erythromycin	1409019-02	1
Fiebig	Erythromycin	1607038-02	1
Fiebig	Erythromycin	1705038	1
Fiebig	Erythromycin	17088005	2
Fiebig	Erythromycin	19L18-F02-367780	1
Fiebig05.2021	Erythromycin	1607038-02	1
Finteler Apotheke	Erythromycin	1607038-02	1
Fragon/ Gehe	Erythromycin	20E18-F06-371571	1
Gatt-Koller	Erythromycin	1803029	2
GEHE 21.05.2014	Erythromycin	1308016-01	1
Gehe amax	Erythromycin	16079213	1
Gehe Rostock	Erythromycin	2007017-01	1
Gehe/ EuRho	Erythromycin	2010014-01	2
Gehe//EuRho	Erythromycin	2002018-01	1
Gehe/EuRho	Erythromycin	2002018-01	1
Gehe	Erythromycin	1106036-05	1
Gehe	Erythromycin	11D13-N09	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Erythromycin	12152105	1
Gehe	Erythromycin	12152108	1
Gehe	Erythromycin	12E24-N04	1
Gehe	Erythromycin	1308016-01	1
Gehe	Erythromycin	1308016-02	1
Gehe	Erythromycin	13189001	2
Gehe	Erythromycin	13F12-N21	1
Gehe	Erythromycin	140901901	1
Gehe	Erythromycin	1409019-01	3
Gehe	Erythromycin	1409019-02	2
Gehe	Erythromycin	15042603	1
Gehe	Erythromycin	15042611	1
Gehe	Erythromycin	15042705	1
Gehe	Erythromycin	150803401	1
Gehe	Erythromycin	1508034-01	1
Gehe	Erythromycin	15245004	1
Gehe	Erythromycin	1607038-01	2
gehe	Erythromycin	1607038-02	2
Gehe	Erythromycin	1607038-02	5
Gehe	Erythromycin	16079204	1
GEHE	Erythromycin	16079208	1
Gehe	Erythromycin	16079209	1
GEHE	Erythromycin	16079213	2
Gehe	Erythromycin	16079505	1
Gehe	Erythromycin	16079510	1
GEHE	Erythromycin	16079512	1
GEHE	Erythromycin	16079609	2
Gehe	Erythromycin	16G06-B03	1
Gehe	Erythromycin	16J24-B10-336735	1
Gehe	Erythromycin	1705038-02	1
Gehe	Erythromycin	1705038-03	1
GEHE	Erythromycin	17088008	1
Gehe	Erythromycin	17088010	1
GEHE	Erythromycin	17088203	2
Gehe	Erythromycin	17088204	1
Gehe	Erythromycin	17088210	1
Gehe	Erythromycin	18096202	1
GEHE	Erythromycin	18096210	1
Gehe	Erythromycin	180964003	1
Gehe	Erythromycin	1811019-01	1
Gehe	Erythromycin	18F05-B01-352501	1
Gehe	Erythromycin	18F05-B01-358088	1
Gehe	Erythromycin	1906032-01	1
Gehe	Erythromycin	19C21-B03-361400	1
Gehe	Erythromycin	19C21-B03-361401	1
Gehe	Erythromycin	19C21-B03-361725	2
Gehe	Erythromycin	19L18-F02-36778	1
Gehe	Erythromycin	20002259007	3
Gehe	Erythromycin	20003732002	1
Gehe	Erythromycin	20003732010	1
Gehe	Erythromycin	2002018-01	1
Gehe	Erythromycin	2007017-01	2
Gehe	Erythromycin	2010014-01	1
Gehe	Erythromycin	20E18-F06-372103	1
Gehe	Erythromycin	21A26-F01	1
GEHE	Erythromycin	21I13-B02-213865	1
Gehe	Erythromycin	22001550002	1
GEHE	Erythromycin	22001550002	1
Gehe	Erythromycin	22002200001	1
Gehe	Erythromycin	22002200003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Erythromycin	22002202003	1
GEHE	Erythromycin	2301053-01	3
Gehe	Erythromycin	2308010-01	2
Gehe	Erythromycin	3D200P	1
Gehe	Erythromycin	f02-3677707	1
Geibo	Erythromycin	20002259003	1
Geilenkirchen	Erythromycin	16J24B10-339488	1
Geilenkirchen	Erythromycin	17088210	2
Geilenkirchen	Erythromycin	17088309	1
Geilenkirchen	Erythromycin	18096205	1
Geilenkirchen	Erythromycin	19L18-F02-367780	1
gepepharm GmbH	Erythromycin	13175502	1
GUMO	Erythromycin	19C21-B03-361725	1
GUMO	Erythromycin	19L18-F02-3677708	1
GUMO	Erythromycin	19L18-F02-3687508	1
GUMO	Erythromycin	20E18-F06	1
GUMO	Erythromycin	F02-3677708	1
Gutenberg-Apotheke	Erythromycin	13175608	1
Hedinger	Erythromycin	15245002	2
Ichthyol-Gesellschaft	Erythromycin	161020E/1607038-01	1
Jenapharm/Phönix	Erythromycin	1607036-01	1
JENNE	Erythromycin	18096202	2
Jenne	Erythromycin	20003732007	1
Kehr	Erythromycin	1705038-01	1
Kehr	Erythromycin	21002041010	1
Kehr	Erythromycin	22002200004	2
Kehr	Erythromycin	226001-01	1
Kehr	Erythromycin	2301053-01	1
Klenk	Erythromycin	EB068I14	1
Klosterring	Erythromycin	CEPEB001E18	1
Krieger	Erythromycin	16G06-B03-329150	1
Krieger	Erythromycin	16J24-B10-336735	1
Krieger	Erythromycin	16J24-B10-341876	1
Krieger	Erythromycin	3402	1
L12	Erythromycin	18096203	1
L30	Erythromycin	17088208	1
Lamotte	Erythromycin	18096406	1
Midas	Erythromycin	16079609	1
Mikrobiell	Erythromycin	1705038-01	1
Mömerzheim	Erythromycin	17088001	1
Nachprüfung	Erythromycin	13175810	1
Noweda 23.08.2019	Erythromycin	1811019-01	1
Noweda Taucha	Erythromycin	21002041001	1
Noweda/Euro	Erythromycin	1607038-01	2
Noweda/Fragron	Erythromycin	18F05-B01-359011	1
Noweda/Gehe	Erythromycin	14B06-B35-293508	1
Noweda	Erythromycin	11195411	2
Noweda	Erythromycin	11195413	1
Noweda	Erythromycin	12152108	2
Noweda	Erythromycin	12152201	1
Noweda	Erythromycin	12E24-N04	1
Noweda	Erythromycin	130801602	2
Noweda	Erythromycin	13175603	2
Noweda	Erythromycin	13175608	1
Noweda	Erythromycin	14044006	1
Noweda	Erythromycin	14044114	1
Noweda	Erythromycin	150803401	1
Noweda	Erythromycin	15245101	1
Noweda	Erythromycin	160703801	1
Noweda	Erythromycin	1607038-02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Erythromycin	16079502	1
Noweda	Erythromycin	16079606	1
Noweda	Erythromycin	16J24-B10	1
Noweda	Erythromycin	16J24-B10-329156	1
Noweda	Erythromycin	1705038-02	2
Noweda	Erythromycin	17088001	1
Noweda	Erythromycin	17088003	1
Noweda	Erythromycin	17088004	1
Noweda	Erythromycin	17088013	1
Noweda	Erythromycin	17088208	1
Noweda	Erythromycin	17088404	1
Noweda	Erythromycin	17088405	2
Noweda	Erythromycin	18096201	1
Noweda	Erythromycin	18096203	1
Noweda	Erythromycin	18096302	1
Noweda	Erythromycin	180964001	1
Noweda	Erythromycin	1811019-01	1
Noweda	Erythromycin	1906032-01	3
Noweda	Erythromycin	19C21-B03-361400	1
Noweda	Erythromycin	20002259004	1
Noweda	Erythromycin	20002259006	1
Noweda	Erythromycin	20003731001	2
Noweda	Erythromycin	20003731003	1
Noweda	Erythromycin	20003731004	1
Noweda	Erythromycin	20003731005	1
Noweda	Erythromycin	2010014-01	1
Noweda	Erythromycin	20I07-F06-375516	1
Noweda	Erythromycin	21002041004	7
Noweda	Erythromycin	220022000002	1
Noweda	Erythromycin	2206001-01	3
Noweda	Erythromycin	23D27-B01-227929	1
NOWEDA	Erythromycin	23D27-B01-227929	2
Noweda	Erythromycin	24C25-B34-001113	2
Noweda	Erythromycin	P2019/92	1
Noweda12/2025	Erythromycin	22002200002	1
Noweda21.04.2015	Erythromycin	14044110	1
OTG/Gehe	Erythromycin	1409019-01	1
Otto Fischar	Erythromycin	16G06-B03-329150	1
Parthe Apotheke	Erythromycin	147/19	1
Parthe Apotheke	Erythromycin	56/21	1
ph.Eur	Erythromycin	2301053-01	1
Ph.Euro/Noweda	Erythromycin	2010015-01	1
Phagron	Erythromycin		1
PHOENIX 08.05.2014	Erythromycin	13175604	1
PHOENIX 08.05.2014	Erythromycin	13175608	2
Phoenix 10.02.2020	Erythromycin	1906032-01	1
Phoenix 28.11.2018	Erythromycin	17088004	1
Phoenix/Cealo	Erythromycin	17088004/0918E-01362	1
Phoenix	Erythromycin	12152201	2
Phoenix	Erythromycin	13175608	1
Phoenix	Erythromycin	14044106	1
Phoenix	Erythromycin	15042609	1
Phoenix	Erythromycin	15042811	1
Phoenix	Erythromycin	16079501	1
Phoenix	Erythromycin	1705038-01	1
Phoenix	Erythromycin	17088403	1
Phoenix	Erythromycin	18096205	1
Phoenix	Erythromycin	18096302	1
Phoenix	Erythromycin	180964003	1
Phoenix	Erythromycin	18096401	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Erythromycin	1906032-01	2
PHOENIX	Erythromycin	19C21-B03	1
Phoenix	Erythromycin	20003731001	1
Phoenix	Erythromycin	20003731004	4
Phoenix	Erythromycin	2002018-01	1
Phoenix	Erythromycin	2007017-01	1
Phoenix	Erythromycin	201001501	1
Phoenix	Erythromycin	21002041014	1
Phoenix	Erythromycin	22002200004	1
Phoenix	Erythromycin	22002203001	1
Phoenix	Erythromycin	23003387001	2
Phoenix	Erythromycin	3104	1
Phoenix	Erythromycin	3207	1
Phönix WE: 23.09.17...	Erythromycin	16079604	1
Phönix Eurho	Erythromycin	2002018-01	1
Phönix Gotha	Erythromycin	18096303	1
Phönix Gotha	Erythromycin	18096403	1
Phönix WE:30.07.2016...	Erythromycin	15245101	1
Phönix	Erythromycin	1205036-02	1
Phönix	Erythromycin	121427016	1
Phönix	Erythromycin	14044201	1
Phönix	Erythromycin	14B06-B35	1
Phönix	Erythromycin	14F13-B02-293511	1
phönix	Erythromycin	15042611	1
phönix	Erythromycin	15042813	1
Phönix	Erythromycin	15042813	2
phönix	Erythromycin	15245101	1
phönix	Erythromycin	16079203	1
Phönix	Erythromycin	16079205	1
Phönix	Erythromycin	16079210	1
Phönix	Erythromycin	1705038-01	3
Phönix	Erythromycin	1705038-03	1
Phönix	Erythromycin	17088002	1
Phonix	Erythromycin	17088005	1
Phönix	Erythromycin	17088301	1
Phönix	Erythromycin	17088306	1
Phönix	Erythromycin	17088404	1
Phönix	Erythromycin	18096209	1
Phönix	Erythromycin	1811019-01	3
PHÖNIX	Erythromycin	1906032	1
Phönix	Erythromycin	1906032-01	4
Phönix	Erythromycin	19C21-B03-361724	2
Phönix	Erythromycin	19118-F02-367779	1
Phönix	Erythromycin	200202018-01	1
Phönix	Erythromycin	200952209	1
Phönix	Erythromycin	2010014-01	1
PHÖNIX	Erythromycin	2010014-01	1
Phönix	Erythromycin	2010015-01	1
Phönix	Erythromycin	20E18-F06-372103	1
Phönix	Erythromycin	21002041009	1
Phönix	Erythromycin	21002041010	1
Phönix	Erythromycin	22001550002	1
Phönix	Erythromycin	22002199001	1
Phönix	Erythromycin	22002200002	2
Phönix	Erythromycin	22002200004	4
Phönix	Erythromycin	22002200005	1
Phönix	Erythromycin	23D27-B01-227928	1
Rondell Apotheke	Erythromycin	15042803	1
Röntgen	Erythromycin	1811019-01	4
Röntgen	Erythromycin	2002018-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Röntgen	Erythromycin	2007017-01	1
Sanacopr	Erythromycin		1
Sanacorp/apo-ident	Erythromycin	1705038-03	1
Sanacorp/EuRho	Erythromycin	17088306	1
Sanacorp	Erythromycin		1
Sanacorp	Erythromycin	1106036-04	1
Sanacorp	Erythromycin	1205035-02	1
Sanacorp	Erythromycin	12152202	1
Sanacorp	Erythromycin	12156208	1
Sanacorp	Erythromycin	1308016-01	1
Sanacorp	Erythromycin	1308016-02	1
Sanacorp	Erythromycin	13H22-N07	1
Sanacorp	Erythromycin	1409019-01	1
Sanacorp	Erythromycin	16079612	1
Sanacorp	Erythromycin	16J24-B10	2
Sanacorp	Erythromycin	16J24B10-338559	1
Sanacorp	Erythromycin	16J24-B10-338559	1
Sanacorp	Erythromycin	1705038-03	1
Sanacorp	Erythromycin	17088002	1
Sanacorp	Erythromycin	17088010	1
Sanacorp	Erythromycin	170880403	1
Sanacorp	Erythromycin	17088203	2
Sanacorp	Erythromycin	17088302	1
Sanacorp	Erythromycin	17088402	1
Sanacorp	Erythromycin	17088404	1
Sanacorp	Erythromycin	18096204	1
Sanacorp	Erythromycin	18096210	1
Sanacorp	Erythromycin	18096404	1
Sanacorp	Erythromycin	18096405	1
sanacorp	Erythromycin	18096406	1
Sanacorp	Erythromycin	181101901	1
Sanacorp	Erythromycin	18F05-B01-350908	2
sanacorp	Erythromycin	1906032-01	1
Sanacorp	Erythromycin	1906032-01	1
Sanacorp	Erythromycin	19C21-B03	1
Sanacorp	Erythromycin	19C21-B03-361401	1
Sanacorp	Erythromycin	19C21-B03-361725	1
Sanacorp	Erythromycin	19L18-F02-368758	1
Sanacorp	Erythromycin	20071017-01	1
Sanacorp	Erythromycin	20100114-01	1
Sanacorp	Erythromycin	2010014-02	1
Sanacorp	Erythromycin	20E18-F06-3721004	1
Sanacorp	Erythromycin	20E18-F06-372104	1
Sanacorp	Erythromycin	21002041004	1
Sanacorp	Erythromycin	21002041014	1
Sanacorp	Erythromycin	21002046001	1
Sanacorp	Erythromycin	21f02-f02-379295	1
Sanacorp	Erythromycin	21I13-B02-213865	1
Sanacorp	Erythromycin	22001550005	2
Sanacorp	Erythromycin	2206001-01	1
Sanacorp	Erythromycin	2301053-01	1
Sanacorp	Erythromycin	23H23-B04-231446	2
Sanacorp	Erythromycin	23H23-B04-236846	1
Sanacorp	Erythromycin	31K190P	1
Sanacorp	Erythromycin	59/AKD51	1
Sanacorp	Erythromycin	60/AKD52	1
Sanacorp;19.03.15;30,50EUR	Erythromycin	1409019-01	1
Sm Biomed / Gehe	Erythromycin	15245002	1
Sm Biomed / Gehe	Erythromycin	16079202	1
Sm Biomed / Gehe	Erythromycin	17088013	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
SM Biomed Sdn Bhd/Phoenix	Erythromycin	2010015-01	1
SM Biomed Sdn. Bhd	Erythromycin	20020018-01	1
SM Biomed Sdn	Erythromycin	18096405	1
SM Biomed/Noweda	Erythromycin	EBD/20-003	1
SM Biomed/Phoenix	Erythromycin	EBD/18-003	2
Spangro	Erythromycin	16079205	1
Spangro	Erythromycin	16G06-B-03-329151	1
Spangro_21.05.2019	Erythromycin	1705038-03	1
Unisan	Erythromycin	140901902	1
VDL	Erythromycin	11195407	1
VDL	Erythromycin	160703801	1
wepa	Erythromycin	2206001-01	1
Wolff/AHD	Erythromycin	15245004	1

- 229 747 spectra from 1515 *Apo-Ident* customers from a total of 48 315 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Erythromycin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Erythromycin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	460	0	152 502
Type B	0	840	0	201 244
Type C	0	6167	153	229 747

The substance/substance group *Erythromycin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6957 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2857 %)
Type C	100.0000 % (> 99.9007 %)	97.5791 % (> 97.5316 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21056	21890	11.02	120.94
21323	22438	6.06	121.76
21651	21651	0.00	137.31
21669	21651	14.77	127.63
21890	21890	0.00	123.28
22438	22438	0.00	123.28
22832	22832	0.00	120.52
23438	23438	0.00	120.22
24420	24420	0.00	138.35

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Escin, water-soluble**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20377-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Escin, water-soluble; Aescinum solubile

Special notes

When selecting the *Escin, water-soluble* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Escin, water-soluble	7	3	3

Second-stage model

For differentiation of the substance/substance group *Escin, water-soluble* the following second-stage model is used:

- Submodel 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Escin, water-soluble* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prednisolon dihydrogen phosphate di…	48.99	–
Riboflavin sodium phosphate hydrate	76.07	–
⋮	⋮	⋮
Mometasone furoate	>50	68.48
Magnesium hydrogen citrate	>50	86.49
Hydrocortisone	>50	94.33
Atropine sulfate	>50	120.90
Quinoline yellow	>50	177.01
Potassium sorbate	>50	263.24
Saccharin sodium	>50	263.65
Calcium orotate dihydrate	>50	387.40
Propranolol hydrochloride	>50	562.70
Phenytoin	>50	906.19

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Escin, water-soluble* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Escin, water-soluble*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Escin, water-soluble	1310020-01	21238	40	AR-15-FG-005777-01
Euro OTC	Escin, water-soluble	1506038	21838	60	20150708*
Euro OTC	Escin, water-soluble	1605021	22684	40	20160609*
Euro OTC	Escin, water-soluble	2009019	25410	40	20201009*
Euro OTC	Escin, water-soluble	2106010	25707	50	20210715*
Fagron	Escin, water-soluble	12K22-N13	21237	40	20121127
Fagron	Escin, water-soluble	12I07-B40-306607	22610	40	1610369

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 310 spectra of 7 reference samples from the substance/substance group *Escin, water-soluble*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 652 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Escin, water-soluble*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Escin, water-soluble	1612012	22988	40
Euro OTC	Escin, water-soluble	1807015-01	24187	40
Euro OTC	Escin, water-soluble	1911023	24939	40

- 201 964 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 3 *Apo-Ident* customers from 4 batches from the substance/substance group *Escin, water-soluble*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Escin, water-soluble	1108038	1
Euro OTC	Escin, water-soluble	1310020-01	1
Euro OTC	Escin, water-soluble	1612012-01	3
Fagron	Escin, water-soluble	30691/M3	1

- 236 061 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Escin, water-soluble* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Escin, water-soluble* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	310	0	152 652
Type B	0	120	0	201 964
Type C	0	6	0	236 061

The substance/substance group *Escin, water-soluble* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0645 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21237	21238	6.88	112.11
21238	21238	0.00	106.44
21838	21838	0.00	126.94
22610	22610	0.00	115.65
22684	22684	0.00	121.82
25410	25410	0.00	117.02
25707	25707	0.00	127.23

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Estradiol benzoate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20098-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Estradiol benzoate; Estradioli benzoas

Special notes

When selecting the *Estradiol benzoate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Estradiol benzoate	7	5	133

Second-stage model

For differentiation of the substance/substance group *Estradiol benzoate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Estradiol benzoate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	152.15	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Estradiol benzoate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Estradiol benzoate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Estradiol benzoate	15078608	23218	40	20150415
Caelo	Estradiol benzoate	181444	24254	40	20180614*
Caelo	Estradiol benzoate	21004177006	26314	40	20220112
Caelo	Estradiol benzoate	21004177006	26314SI	40	20220112
Euro OTC	Estradiol benzoate	1301006-02	21290	40	1507405
Euro OTC	Estradiol benzoate	1507009	21869	60	0000010566
Euro OTC	Estradiol benzoate	1507009	21869SI	60	0000010566
Fagron	Estradiol benzoate	12H02-N02	20889	40	20120817
Fagron	Estradiol benzoate	12H02-N02	20889SI	60	20120817
Fagron	Estradiol benzoate	14B20-B02	21257	40	20140327
Fagron	Estradiol benzoate	14B20-B02	21257SI	60	20140327

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 520 spectra of 11 reference samples from the substance/substance group *Estradiol benzoate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 442 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 440 spectra of 11 reference samples from the substance/substance group *Estradiol benzoate*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Estradiol benzoate	13277607	21324	40
Euro OTC	Estradiol benzoate	1611004	22873	40
Euro OTC	Estradiol benzoate	1412033	24139	40
Euro OTC	Estradiol benzoate	2001032	25113	40
Fagron	Estradiol benzoate	24B26-B06-228380	27184	40
Caelo	Estradiol benzoate	15078608	23218SI†	40
Caelo	Estradiol benzoate	181444	24254SI†	40
Euro OTC	Estradiol benzoate	1611004	22873SI	40
Euro OTC	Estradiol benzoate	1412033	24139SI	40
Euro OTC	Estradiol benzoate	2001032	25113SI	40
Fagron	Estradiol benzoate	24B26-B06-228380	27184SI	40

- 201 644 spectra from a total of 4038 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 884 spectra from 547 *Apo-Ident* customers from 142 batches from the substance/substance group *Estradiol benzoate*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 132 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Estradiol benzoate	2001032	1
	Estradiol benzoate	2001032-03	2
	Estradiol benzoate	21004177005	1
	Estradiol benzoate	2300012002	1
	Estradiol benzoate	23000121002	4
	Estradiol benzoate	23000121003	7
	Estradiol benzoate	23000121005	1
	Estradiol benzoate	3919E-01946	1
A.H. 07.06.13 ek: 24,14EUR	Estradiol benzoate	1201019-02	1
AHC	Estradiol benzoate	18144408	1
AHD	Estradiol benzoate	14B20-B02-292001	1
AHD	Estradiol benzoate	1611004-02	1
AHD	Estradiol benzoate	18144404	1
aliance healthcare 5...	Estradiol benzoate	10118576	1
Alliance Healthcare	Estradiol benzoate	1301006-01	1
apo-ident	Estradiol benzoate	18144405	1
Bayer Pharma AG / Noweda	Estradiol benzoate	14B20-B02	1
Bayer Pharma/Noweda	Estradiol benzoate	14B20-B02-292001	1
Bayer-Schering	Estradiol benzoate	1007037-03	1
Caelo	Estradiol benzoate		4
Caelo	Estradiol benzoate	10124909	5
Caelo	Estradiol benzoate	10124912	1
Caelo	Estradiol benzoate	10124915	2
Caelo	Estradiol benzoate	10124918	2
Caelo	Estradiol benzoate	10124919	1
Caelo	Estradiol benzoate	10124921	1
Caelo	Estradiol benzoate	1100417	1
Caelo	Estradiol benzoate	111004-02	1
Caelo	Estradiol benzoate	1149	1
Caelo	Estradiol benzoate	1201019-02	1
Caelo	Estradiol benzoate	12255904	10
Caelo	Estradiol benzoate	12255905	10
Caelo	Estradiol benzoate	1301006-02	1
Caelo	Estradiol benzoate	13276401	6
Caelo	Estradiol benzoate	13277602	8
Caelo	Estradiol benzoate	13277603	2
Caelo	Estradiol benzoate	13277605	4
Caelo	Estradiol benzoate	13277607	3
Caelo	Estradiol benzoate	1401001-01	1
Caelo	Estradiol benzoate	1412033-02	1
Caelo	Estradiol benzoate	1507009-01	1
Caelo	Estradiol benzoate	1507806	1
Caelo	Estradiol benzoate	15078602	8
Caelo	Estradiol benzoate	15078603	22
Caelo	Estradiol benzoate	15078604	21
Caelo	Estradiol benzoate	15078606	6
Caelo	Estradiol benzoate	15078608	16
Caelo	Estradiol benzoate	15078609	1
Caelo	Estradiol benzoate	150918EB	1
Caelo	Estradiol benzoate	15C10B04305523	1
Caelo	Estradiol benzoate	15C10-B04-305523	2
Caelo	Estradiol benzoate	16003701	7
Caelo	Estradiol benzoate	16003702	7
Caelo	Estradiol benzoate	16003707	22
Caelo	Estradiol benzoate	1611004-01	1
Caelo	Estradiol benzoate	1611004-02	2
Caelo	Estradiol benzoate	17357602	8

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Estradiol benzoate	17357604	2
Caelo	Estradiol benzoate	17357605	12
Caelo	Estradiol benzoate	1814404	1
Caelo	Estradiol benzoate	1814405	1
Caelo	Estradiol benzoate	1814408	1
Caelo	Estradiol benzoate	18144402	23
Caelo	Estradiol benzoate	18144404	19
Caelo	Estradiol benzoate	18144405	31
Caelo	Estradiol benzoate	18144406	17
Caelo	Estradiol benzoate	18144406P-191101-1	1
Caelo	Estradiol benzoate	18144408	22
Caelo	Estradiol benzoate	181444404	1
Caelo	Estradiol benzoate	181444405	1
Caelo	Estradiol benzoate	181444406	1
Caelo	Estradiol benzoate	1844406	1
Caelo	Estradiol benzoate	200000164001	2
Caelo	Estradiol benzoate	20000164001	53
Caelo	Estradiol benzoate	2000016401	2
Caelo	Estradiol benzoate	2000164001	1
Caelo	Estradiol benzoate	2001032-01	1
Caelo	Estradiol benzoate	21000144002	1
Caelo	Estradiol benzoate	21000145001	18
Caelo	Estradiol benzoate	21000145003	8
Caelo	Estradiol benzoate	21004177003	18
Caelo	Estradiol benzoate	21004177004	4
Caelo	Estradiol benzoate	21004177005	10
Caelo	Estradiol benzoate	21004177006	11
Caelo	Estradiol benzoate	21004177008	11
Caelo	Estradiol benzoate	21121204	1
Caelo	Estradiol benzoate	227051-08-08	1
Caelo	Estradiol benzoate	23000121002	3
Caelo	Estradiol benzoate	32308779	1
Caelo	Estradiol benzoate	6091305	1
Caelo	Estradiol benzoate	81403700	1
Caelo	Estradiol benzoate	84303830	2
Caelo	Estradiol benzoate	92137389	1
Caelo	Estradiol benzoate	eucerin	1
Caesar & Loretz GmbH...	Estradiol benzoate	21004177003	1
Caesar & Loretz GmbH...	Estradiol benzoate	18144404	1
Caesar & Loretz GmbH...	Estradiol benzoate	21004177008	1
Caesar & Loretz GmbH...	Estradiol benzoate	21000145003	1
Caesar & Loretz GmbH/AHD	Estradiol benzoate	21004177006	1
Caesar & Loretz GmbH...	Estradiol benzoate	18144404	1
Caesar & Loretz GmbH...	Estradiol benzoate	21000145001	1
Caesar & Loretz GmbH/Gehe	Estradiol benzoate	18144405	1
Caesar & Loretz GmbH/GEHE	Estradiol benzoate	18144405	1
Caesar & Loretz GmbH/GEHE	Estradiol benzoate	18144406	1
Caesar & Loretz GmbH/Gehe	Estradiol benzoate	20000164001	1
Caesar & Loretz GmbH/Gehe	Estradiol benzoate	21004177004	2
Caesar & Loretz GmbH...	Estradiol benzoate	20000164001	1
Caesar & Loretz GmbH/Kehr	Estradiol benzoate	20000164001	1
Caesar & Loretz GmbH...	Estradiol benzoate	18144402	1
Caesar & Loretz GmbH...	Estradiol benzoate	21000145001	1
Caesar & Loretz GmbH/Ph	Estradiol benzoate	18144408	1
Caesar & Loretz GmbH...	Estradiol benzoate	20000164001	1
Caesar & Loretz GmbH...	Estradiol benzoate	18144404	1
Caesar & Loretz GmbH...	Estradiol benzoate	21004177005	1
Caesar & Loretz GmbH...	Estradiol benzoate	21004177003	1
Caesar & Loretz GmbH	Estradiol benzoate	17357605	4
Caesar & Loretz GmbH	Estradiol benzoate	18144402	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Estradiol benzoate	18144405	12
Caesar & Loretz GmbH	Estradiol benzoate	18144406	9
Caesar & Loretz GmbH	Estradiol benzoate	18144408	4
Caesar & Loretz GmbH	Estradiol benzoate	20000164001	8
Caesar & Loretz GmbH	Estradiol benzoate	21000145001	6
Caesar & Loretz GmbH	Estradiol benzoate	21000145003	3
Caesar & Loretz GmbH	Estradiol benzoate	21004177003	4
Caesar & Loretz GmbH	Estradiol benzoate	21004177004	4
Caesar & Loretz GmbH	Estradiol benzoate	21004177005	3
Caesar & Loretz GmbH	Estradiol benzoate	21004177006	12
Caesar & Loretz GmbH	Estradiol benzoate	21004177008	1
Caesar & Loretz GmbH	Estradiol benzoate	23000121002	2
Caesar & Loretz	Estradiol benzoate	17357605	1
Caesar / Gehe	Estradiol benzoate	16003707	1
Caesar L / Sanacorp	Estradiol benzoate	18144408	1
Caesar&Lorenz / Gehe	Estradiol benzoate	18144405	1
Caesar&Lorenz	Estradiol benzoate	21000145001	1
Cealo/Noweda	Estradiol benzoate	18144405	1
Cealo	Estradiol benzoate	15078604	1
EuRho/Sanacorp	Estradiol benzoate	1201019-02	1
EuRho	Estradiol benzoate	84303830	1
Euro OTC	Estradiol benzoate	1007037-02	1
Euro OTC	Estradiol benzoate	1201019-01	7
Euro OTC	Estradiol benzoate	1201019-02	9
Euro OTC	Estradiol benzoate	121019-01	1
Euro OTC	Estradiol benzoate	130100601	1
Euro OTC	Estradiol benzoate	1301006-01	2
Euro OTC	Estradiol benzoate	1301006-02	11
Euro OTC	Estradiol benzoate	14010001-01	1
Euro OTC	Estradiol benzoate	1401001-01	10
Euro OTC	Estradiol benzoate	140101-01	1
Euro OTC	Estradiol benzoate	1412033-01	9
Euro OTC	Estradiol benzoate	1412033-02	6
Euro OTC	Estradiol benzoate	150700901	2
Euro OTC	Estradiol benzoate	1507009-01	16
Euro OTC	Estradiol benzoate	1507009-01I-0401016	1
Euro OTC	Estradiol benzoate	16003707	1
Euro OTC	Estradiol benzoate	1611004-01	11
Euro OTC	Estradiol benzoate	161100402	2
Euro OTC	Estradiol benzoate	1611004-02	21
Euro OTC	Estradiol benzoate	1611004-028638831	1
Euro OTC	Estradiol benzoate	16110047-02	1
Euro OTC	Estradiol benzoate	16111004-01	1
Euro OTC	Estradiol benzoate	1807161	1
Euro OTC	Estradiol benzoate	2001032-01	15
Euro OTC	Estradiol benzoate	2001032-02	3
Euro OTC	Estradiol benzoate	2001032-03	2
Euro OTC	Estradiol benzoate	21000145003	1
Euro OTC	Estradiol benzoate	8011422	1
Euro OTC	Estradiol benzoate	83101340	1
Euro OTC	Estradiol benzoate	84303830	2
EURO Pharma	Estradiol benzoate	84303830	1
Euro/Krieger	Estradiol benzoate	1611004-02	1
Fagron	Estradiol benzoate	11H01-N12	1
Fagron	Estradiol benzoate	11L23-N01	2
Fagron	Estradiol benzoate	12B08-N05	1
Fagron	Estradiol benzoate	12D20N06	1
Fagron	Estradiol benzoate	12H02-N02	3
Fagron	Estradiol benzoate	12H02-N052	1
Fagron	Estradiol benzoate	12L14-N02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Estradiol benzoate	13/11-N01	2
Fagron	Estradiol benzoate	13C15-B07-288645	1
Fagron	Estradiol benzoate	13I11N01	1
Fagron	Estradiol benzoate	13I11-N01	1
Fagron	Estradiol benzoate	1412033-01	1
Fagron	Estradiol benzoate	14820-B02-294949	1
Fagron	Estradiol benzoate	14B20-B02	3
Fagron	Estradiol benzoate	14B20-B02-2920001	1
Fagron	Estradiol benzoate	14B20-B02-292001	6
Fagron	Estradiol benzoate	14b20-b02-294949	1
Fagron	Estradiol benzoate	14B20-B02-294949	3
Fagron	Estradiol benzoate	15c10-b04-305523	1
Fagron	Estradiol benzoate	15C10-B04-305523	6
Fagron	Estradiol benzoate	15E08-B08	1
Fagron	Estradiol benzoate	15E08-B08-311705	13
Fagron	Estradiol benzoate	17357602	1
Fagron	Estradiol benzoate	17L01-B05-3434714	1
Fagron	Estradiol benzoate	17L01B05343714	1
Fagron	Estradiol benzoate	17L01-B05-343714	4
Fagron	Estradiol benzoate	17L01-B05-348601	1
Fagron	Estradiol benzoate	2001032-01	1
Fagron	Estradiol benzoate	20D16-F08-370349	1
Fagron	Estradiol benzoate	2x12L14-N02	1
Fagron	Estradiol benzoate	81403680	1
Fagron	Estradiol benzoate	81403690	3
Fagron	Estradiol benzoate	83101340	2
Fagron	Estradiol benzoate	84303830	1
Fagron	Estradiol benzoate	84303840	1
Fargon/AHD	Estradiol benzoate	15E08-B08-311705	2
Fiebig	Estradiol benzoate	20000164001	1
Finze	Estradiol benzoate	1003040-01	2
Gehe	Estradiol benzoate	11L23-N01	1
Gehe	Estradiol benzoate	15078606	1
GEHE	Estradiol benzoate	15078609	1
Gehe	Estradiol benzoate	17L01-B05-343714	1
Gehe	Estradiol benzoate	18144405	2
Gehe	Estradiol benzoate	18144408	1
Gehe	Estradiol benzoate	20000164001	1
Gehe	Estradiol benzoate	2001032-02	1
Gehe	Estradiol benzoate	21004177005	1
Gehe	Estradiol benzoate	23000121002	1
GUMO	Estradiol benzoate	21000145001	1
Jenne/Caesar & Loret…	Estradiol benzoate	21004177004	1
Kehr	Estradiol benzoate	18144404	1
Kehr	Estradiol benzoate	23000121003	1
Klenk	Estradiol benzoate	8(18144402)	1
Krieger	Estradiol benzoate	3401	1
Nachprüfung	Estradiol benzoate	123456	1
Noweda	Estradiol benzoate	13277603	1
Noweda	Estradiol benzoate	15078608	1
Noweda	Estradiol benzoate	18144402	1
Noweda	Estradiol benzoate	2001032-01	1
Noweda	Estradiol benzoate	21000145001	2
Noweda	Estradiol benzoate	21004177003	1
Noweda	Estradiol benzoate	21004177004	1
Phoenix 1.10.2018	Estradiol benzoate	17357602	1
Phoenix WE:20.11.17 …	Estradiol benzoate	16003702	1
Phoenix/Cealo	Estradiol benzoate	1611004-01	1
Phoenix	Estradiol benzoate	15078608	1
Phoenix	Estradiol benzoate	18144402	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Estradiol benzoate	20d16-f08-373007	1
Phoenix	Estradiol benzoate	8638831	1
phönix	Estradiol benzoate	14B20-B02-294949	1
Phönix	Estradiol benzoate	16003707	2
phönix	Estradiol benzoate	21004177004	1
Sanacorp 04.07.19 Ek…	Estradiol benzoate	18144404	1
Sanacorp	Estradiol benzoate	10/AKD24	1
sanacorp	Estradiol benzoate	15078604	1
Sanacorp	Estradiol benzoate	16003707	1
Sanacorp	Estradiol benzoate	17L01-B05	2
Sanacorp	Estradiol benzoate	17L01-B05-343714	1
Sanacorp	Estradiol benzoate	1814402	1
Sanacorp	Estradiol benzoate	21004177005	1
Sanacorp	Estradiol benzoate	23000121002	2
Valdepharm/Phoenix	Estradiol benzoate	ESB002-3E	1
VDl 16.10.14 12,70 euro	Estradiol benzoate		1
VDL	Estradiol benzoate	1507009-01	1
WE:Phönix 21.09.2012	Estradiol benzoate	12B08-N05	1

- 235 183 spectra from 1515 *Apo-Ident* customers from a total of 49 120 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Estradiol benzoate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Estradiol benzoate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	520	0	152 442
Type B	0	440	0	201 644
Type C	0	873	11	235 183

The substance/substance group *Estradiol benzoate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8462 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6364 %)
Type C	100.0000 % (> 99.9007 %)	98.7557 % (> 98.4163 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20889	21290	10.50	215.63
21257	21290	4.39	213.45
21290	21290	0.00	213.66
21869	21869	0.00	217.11
23218	21869	10.39	216.26
24254	24254	0.00	216.07
26314	21869	12.41	216.29

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Estradiol hemihydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20497-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Estradiol hemihydrate; Estradiolum hemihydricum

Special notes

When selecting the *Estradiol hemihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Estradiol hemihydrate	11	27	155

Second-stage model

For differentiation of the substance/substance group *Estradiol hemihydrate* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Estradiol hemihydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	52.45	–
⋮	⋮	⋮
Estriol	>50	20.42
Polymyxin B sulfate	>50	36.54
Bacitracin	>50	41.95
Amphotericin B	>50	53.77
Cyanocobalamin	>50	56.99
Riboflavin	>50	58.27
Colistin sulfate	>50	59.92
Nystatin	>50	72.43
Triamcinolone	>50	73.96
alpha-tocopheryl acetate dry concentrate	>50	101.15
Calcium glycerophosphate	>50	110.81
Selenium yeast	>50	127.57
Methylcobalamin	>50	135.87
Calcium pantothenate	>50	137.78
Gelatine, white	>50	164.68
SyrSpend® SF Alka	>50	185.24
Hyoscine hydrobromide	>50	194.33
Tosylchloramide sodium	>50	201.04
SyrSpend® SF pH4 neo (Maize starch)	>50	211.67
Carmellose sodium	>50	220.24
Rice starch	>50	298.95
Oxalic acid	>50	338.81
Corn starch	>50	347.66
Acacia, dried dispersion	>50	498.96
Wheat starch	>50	507.84
SyrSpend® SF pH4	>50	508.23
Maltodextrin	>50	533.89
Potato starch	>50	594.92
Fructose	>50	715.93

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Estradiol hemihydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Estradiol hemihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Estradiol hemihydrate	12268016	21302	40	1410502
Caelo	Estradiol hemihydrate	13285802	21499	60	20130913
Caelo	Estradiol hemihydrate	13285802	21500	60	1510622
Caelo	Estradiol hemihydrate	13285802	21501	20	20130913
Caelo	Estradiol hemihydrate	13285802	21502	20	20130913
Caelo	Estradiol hemihydrate	13285802	21503	20	20130913
Caelo	Estradiol hemihydrate	13285802	21504	20	20130913
Caelo	Estradiol hemihydrate	13285802	21505	20	20130913
Caelo	Estradiol hemihydrate	13285802	21506	20	20130913
Caelo	Estradiol hemihydrate	13285802	21507	20	20130913
Caelo	Estradiol hemihydrate	13285802	21508	60	1410504
Euro OTC	Estradiol hemihydrate	1208022-01	21291	40	20121012
Euro OTC	Estradiol hemihydrate	1507013	21847	60	1510623
Euro OTC	Estradiol hemihydrate	1507013	21847SI	60	1510623
Euro OTC	Estradiol hemihydrate	1510039	21945	60	20151103*
Euro OTC	Estradiol hemihydrate	1510039	21945SI	89	20151103*
Euro OTC	Estradiol hemihydrate	1601017	22307	45	20160122*
Euro OTC	Estradiol hemihydrate	1612008	22913	40	20170117*
Euro OTC	Estradiol hemihydrate	1612008	22913SI	40	20170117*
Euro OTC	Estradiol hemihydrate	2009029	25402	40	20201012*
Euro OTC	Estradiol hemihydrate	2103014	25608	40	20210406*
Euro OTC	Estradiol hemihydrate	2103014	25608SI	40	20210406*
Fagron	Estradiol hemihydrate	14G24-B04-297404	21667	55	20140825
Fagron	Estradiol hemihydrate	16H04-B01-328738	23184	40	20160915

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1009 spectra of 24 reference samples from the substance/substance group *Estradiol hemihydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.
- 151 953 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 2464 spectra of 65 reference samples from the substance/substance group *Estradiol hemihydrate*.
- Among them are spectra of independent samples from 27 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Estradiol hemihydrate	170582	23339	40
Caelo	Estradiol hemihydrate	181443	24257	40
Caelo	Estradiol hemihydrate	21003879006	26315	40
Euro OTC	Estradiol hemihydrate	1607003	22712	40
Euro OTC	Estradiol hemihydrate	1612008-01	23099	40
Euro OTC	Estradiol hemihydrate	1705018	23431	40
Euro OTC	Estradiol hemihydrate	1710031	23779	40
Euro OTC	Estradiol hemihydrate	1802013	24083	40
Euro OTC	Estradiol hemihydrate	1802012	24086	40
Euro OTC	Estradiol hemihydrate	1809022	24319	40
Euro OTC	Estradiol hemihydrate	1808032	24322	40
Euro OTC	Estradiol hemihydrate	1905001	24639	40
Euro OTC	Estradiol hemihydrate	1906013	24772	40
Euro OTC	Estradiol hemihydrate	1910006	24973	40
Euro OTC	Estradiol hemihydrate	1911010	24983	40
Euro OTC	Estradiol hemihydrate	2002008	25108	40
Euro OTC	Estradiol hemihydrate	2002009	25109	40
Euro OTC	Estradiol hemihydrate	2002007	25114	40
Euro OTC	Estradiol hemihydrate	2006023	25257	40
Euro OTC	Estradiol hemihydrate	2006024	25266	40
Euro OTC	Estradiol hemihydrate	2006022	25284	40
Euro OTC	Estradiol hemihydrate	2009028	25403	40
Euro OTC	Estradiol hemihydrate	2201041	25966	40
Euro OTC	Estradiol hemihydrate	2303010	26656	40
Euro OTC	Estradiol hemihydrate	2405012	27278	40
Fagron	Estradiol hemihydrate	13K22-N01	21263	40
Fagron	Estradiol hemihydrate	22I23-B01-225111	26374	40
Caelo	Estradiol hemihydrate	13285802	21499SI†	60
Caelo	Estradiol hemihydrate	13285802	21500SI†	60
Caelo	Estradiol hemihydrate	13285802	21501SI†	20
Caelo	Estradiol hemihydrate	13285802	21502SI†	20
Caelo	Estradiol hemihydrate	13285802	21503SI†	20
Caelo	Estradiol hemihydrate	13285802	21504SI†	20
Caelo	Estradiol hemihydrate	13285802	21505SI†	20
Caelo	Estradiol hemihydrate	13285802	21506SI†	20
Caelo	Estradiol hemihydrate	13285802	21507SI†	20
Caelo	Estradiol hemihydrate	170582	23339SI	30
Caelo	Estradiol hemihydrate	181443	24257SI	40
Caelo	Estradiol hemihydrate	21003879006	26315SI	40
Euro OTC	Estradiol hemihydrate	1601017	22307SI†	45
Euro OTC	Estradiol hemihydrate	1607003	22712SI	40
Euro OTC	Estradiol hemihydrate	1612008-01	23099SI	30
Euro OTC	Estradiol hemihydrate	1705018	23431SI	30
Euro OTC	Estradiol hemihydrate	1710031	23779SI	40

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Estradiol hemihydrate	1802013	24083SI	40
Euro OTC	Estradiol hemihydrate	1802012	24086SI	40
Euro OTC	Estradiol hemihydrate	1809022	24319SI	40
Euro OTC	Estradiol hemihydrate	1808032	24322SI	40
Euro OTC	Estradiol hemihydrate	1905001	24639SI	40
Euro OTC	Estradiol hemihydrate	1906013	24772SI	39
Euro OTC	Estradiol hemihydrate	1910006	24973SI	40
Euro OTC	Estradiol hemihydrate	1911010	24983SI	40
Euro OTC	Estradiol hemihydrate	2002008	25108SI	40
Euro OTC	Estradiol hemihydrate	2002009	25109SI	40
Euro OTC	Estradiol hemihydrate	2002007	25114SI	40
Euro OTC	Estradiol hemihydrate	2006023	25257SI	40
Euro OTC	Estradiol hemihydrate	2006024	25266SI	40
Euro OTC	Estradiol hemihydrate	2006022	25284SI	40
Euro OTC	Estradiol hemihydrate	2009029	25402SI[†]	40
Euro OTC	Estradiol hemihydrate	2009028	25403SI	40
Euro OTC	Estradiol hemihydrate	2201041	25966SI	40
Euro OTC	Estradiol hemihydrate	2303010	26656SI	40
Euro OTC	Estradiol hemihydrate	2405012	27278SI	40
Fagron	Estradiol hemihydrate	16H04-B01-328738	23184SI[†]	30
Fagron	Estradiol hemihydrate	22I23-B01-225111	26374SI	40

- 199 620 spectra from a total of 4014 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 597 spectra from 220 *Apo-Ident* customers from 164 batches from the substance/substance group *Estradiol hemihydrate*.

- Among them are spectra of independent samples from 155 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Estradiol hemihydrate	21003879006	2
	Estradiol hemihydrate	21003879009	2
	Estradiol hemihydrate	2103014-02	1
	Estradiol hemihydrate	22123-B01	1
	Estradiol hemihydrate	23000120001	2
	Estradiol hemihydrate	2300020001	1
Anzag; 12.72EUR; 7.10.2015	Estradiol hemihydrate	15038004	1
Audor Pharma	Estradiol hemihydrate	1911010-01	1
Bayer Pharma AG	Estradiol hemihydrate	1411024-01	2
Bayer Pharma	Estradiol hemihydrate	13K22-N01	2
Caelo	Estradiol hemihydrate	108082101	1
Caelo	Estradiol hemihydrate	11078104	1
Caelo	Estradiol hemihydrate	11078105	1
Caelo	Estradiol hemihydrate	11078113	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Estradiol hemihydrate	12172003	2
Caelo	Estradiol hemihydrate	12268003	1
Caelo	Estradiol hemihydrate	12268012	5
Caelo	Estradiol hemihydrate	12F29-N03	1
Caelo	Estradiol hemihydrate	13285801	1
Caelo	Estradiol hemihydrate	13285802	4
Caelo	Estradiol hemihydrate	13285804	1
Caelo	Estradiol hemihydrate	13285811	4
Caelo	Estradiol hemihydrate	13K22-N01	1
Caelo	Estradiol hemihydrate	15038004	5
Caelo	Estradiol hemihydrate	1503801	1
Caelo	Estradiol hemihydrate	15038010	2
Caelo	Estradiol hemihydrate	15038014	2
Caelo	Estradiol hemihydrate	15038016	2
Caelo	Estradiol hemihydrate	15385406	1
Caelo	Estradiol hemihydrate	15385410	4
Caelo	Estradiol hemihydrate	15385411	1
Caelo	Estradiol hemihydrate	15385415	2
Caelo	Estradiol hemihydrate	15D01-B02-319032	1
Caelo	Estradiol hemihydrate	1601017-01	5
Caelo	Estradiol hemihydrate	1612008-01	1
Caelo	Estradiol hemihydrate	1705018-01	3
Caelo	Estradiol hemihydrate	17058205	4
Caelo	Estradiol hemihydrate	18082101	3
Caelo	Estradiol hemihydrate	18082101P-180904-1	1
Caelo	Estradiol hemihydrate	18082103	1
Caelo	Estradiol hemihydrate	18082104	4
Caelo	Estradiol hemihydrate	18082105	6
Caelo	Estradiol hemihydrate	18144306	2
Caelo	Estradiol hemihydrate	18144308	1
Caelo	Estradiol hemihydrate	18144309	3
Caelo	Estradiol hemihydrate	18144314	3
Caelo	Estradiol hemihydrate	18F18-B01-351946	1
Caelo	Estradiol hemihydrate	19051501	1
Caelo	Estradiol hemihydrate	193089002	3
Caelo	Estradiol hemihydrate	193089003	1
Caelo	Estradiol hemihydrate	193089007	5
Caelo	Estradiol hemihydrate	193089010	5
Caelo	Estradiol hemihydrate	193089011	2
Caelo	Estradiol hemihydrate	19308910	1
Caelo	Estradiol hemihydrate	20I18-F03-374511	1
Caelo	Estradiol hemihydrate	21000148001	7
Caelo	Estradiol hemihydrate	21003879001	1
Caelo	Estradiol hemihydrate	21003879006	3
Caelo	Estradiol hemihydrate	22101301	1
Caelo	Estradiol hemihydrate	84201560	1
Caelo	Estradiol hemihydrate	9248916	2
Caesar & Loretz GmbH...	Estradiol hemihydrate	18144309	1
Caesar & Loretz GmbH...	Estradiol hemihydrate	21003879006	1
Caesar & Loretz GmbH...	Estradiol hemihydrate	193089011	1
Caesar & Loretz GmbH/Sana	Estradiol hemihydrate	193089010	1
Caesar & Loretz GmbH...	Estradiol hemihydrate	193089011	1
Caesar & Loretz GmbH	Estradiol hemihydrate	15385415	1
Caesar & Loretz GmbH	Estradiol hemihydrate	18082104	5
Caesar & Loretz GmbH	Estradiol hemihydrate	18082105	1
Caesar & Loretz GmbH	Estradiol hemihydrate	18144306	2
Caesar & Loretz GmbH	Estradiol hemihydrate	18144309	1
Caesar & Loretz GmbH	Estradiol hemihydrate	193089002	1
Caesar & Loretz GmbH	Estradiol hemihydrate	193089006	1
Caesar & Loretz GmbH	Estradiol hemihydrate	193089007	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Estradiol hemihydrate	193089011	1
Caesar & Loretz GmbH	Estradiol hemihydrate	21000148001	2
Caesar & Loretz GmbH	Estradiol hemihydrate	21000148003	1
Caesar & Loretz GmbH	Estradiol hemihydrate	21003879006	5
ESD	Estradiol hemihydrate	ESD-20010	1
EuRho/Sanacorp	Estradiol hemihydrate	1911010-01	1
Eurho	Estradiol hemihydrate	2002007-01	1
Euro OTC	Estradiol hemihydrate	1308003-01	2
Euro OTC	Estradiol hemihydrate	1374814	1
Euro OTC	Estradiol hemihydrate	1404030-01	1
Euro OTC	Estradiol hemihydrate	1411024-01	2
Euro OTC	Estradiol hemihydrate	1504034-01	1
Euro OTC	Estradiol hemihydrate	1507013-01	1
Euro OTC	Estradiol hemihydrate	1510039-01	11
Euro OTC	Estradiol hemihydrate	15D01-B02	1
Euro OTC	Estradiol hemihydrate	1601017-01	10
Euro OTC	Estradiol hemihydrate	1607003-01	29
Euro OTC	Estradiol hemihydrate	1607003-0101374814	1
Euro OTC	Estradiol hemihydrate	1612008_01	1
Euro OTC	Estradiol hemihydrate	1612008-01	26
Euro OTC	Estradiol hemihydrate	1705018-01	18
Euro OTC	Estradiol hemihydrate	17058205	1
Euro OTC	Estradiol hemihydrate	1802012-01	1
Euro OTC	Estradiol hemihydrate	1802013-01	3
Euro OTC	Estradiol hemihydrate	1808032-01	23
Euro OTC	Estradiol hemihydrate	1809022-01	7
Euro OTC	Estradiol hemihydrate	180902202	1
Euro OTC	Estradiol hemihydrate	1809022-02	6
Euro OTC	Estradiol hemihydrate	1906013-01	3
Euro OTC	Estradiol hemihydrate	1910006-01	4
Euro OTC	Estradiol hemihydrate	1911010-01	4
Euro OTC	Estradiol hemihydrate	2002009-01	4
Euro OTC	Estradiol hemihydrate	2006022-01	15
Euro OTC	Estradiol hemihydrate	2006023-01	12
Euro OTC	Estradiol hemihydrate	2006024-01	14
Euro OTC	Estradiol hemihydrate	20090028-01	1
Euro OTC	Estradiol hemihydrate	2009028-01	18
Euro OTC	Estradiol hemihydrate	2009029	10
Euro OTC	Estradiol hemihydrate	2009029-01	20
Euro OTC	Estradiol hemihydrate	2103014-0	2
Euro OTC	Estradiol hemihydrate	210301401	1
Euro OTC	Estradiol hemihydrate	2103014-01	19
Euro OTC	Estradiol hemihydrate	2201041-01	8
Euro OTC	Estradiol hemihydrate	2303010-01	6
Euro OTC	Estradiol hemihydrate	2405012-01	1
Euro OTC	Estradiol hemihydrate	27061714	1
Euro OTC	Estradiol hemihydrate	701634	1
Euro/ Phönix	Estradiol hemihydrate	3417M-02845	1
Fagron	Estradiol hemihydrate		1
Fagron	Estradiol hemihydrate	11031401	1
Fagron	Estradiol hemihydrate	11A21-N01	1
Fagron	Estradiol hemihydrate	11H23-N02	1
Fagron	Estradiol hemihydrate	12F29-N03	6
Fagron	Estradiol hemihydrate	12L19-N07	7
Fagron	Estradiol hemihydrate	12L29-N07	1
Fagron	Estradiol hemihydrate	13E07-N02	4
Fagron	Estradiol hemihydrate	13k22n01	1
Fagron	Estradiol hemihydrate	13K22N01	1
Fagron	Estradiol hemihydrate	13K22-N01	5
Fagron	Estradiol hemihydrate	14G24-B04	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Estradiol hemihydrate	14G24-B04-297402	3
Fagron	Estradiol hemihydrate	14G24-B04-297404	1
Fagron	Estradiol hemihydrate	14G24-B04-297405	1
Fagron	Estradiol hemihydrate	14G24-B04-297406	1
Fagron	Estradiol hemihydrate	14G24-B04-302446	3
Fagron	Estradiol hemihydrate	15D01-B02-308190	1
Fagron	Estradiol hemihydrate	15D01-B02-308568	2
Fagron	Estradiol hemihydrate	15D01-B02-312068	3
Fagron	Estradiol hemihydrate	15D01-B02-319032	4
Fagron	Estradiol hemihydrate	16D12-B01-322022	1
Fagron	Estradiol hemihydrate	16D12B01326783	1
Fagron	Estradiol hemihydrate	16D12-B01-326783	6
Fagron	Estradiol hemihydrate	16h04-b01-328738	1
Fagron	Estradiol hemihydrate	16H04-B01-328738	1
Fagron	Estradiol hemihydrate	16h04-b01-334200	1
Fagron	Estradiol hemihydrate	16H04-B01-334200	4
Fagron	Estradiol hemihydrate	16H04-B01-334592	1
Fagron	Estradiol hemihydrate	16h04-b01-337595	1
Fagron	Estradiol hemihydrate	16H04-B01-33795	1
Fagron	Estradiol hemihydrate	16H04-B01-339490	1
Fagron	Estradiol hemihydrate	1802012-01	1
Fagron	Estradiol hemihydrate	1802013-01	3
Fagron	Estradiol hemihydrate	18F18-B01	2
Fagron	Estradiol hemihydrate	18F18-B01-351789	1
Fagron	Estradiol hemihydrate	18F18-B01-351790	1
Fagron	Estradiol hemihydrate	18F18-B01-351946	2
Fagron	Estradiol hemihydrate	18F18-B01-354821	1
Fagron	Estradiol hemihydrate	18F18-B01-355586	1
Fagron	Estradiol hemihydrate	18F18-B01-357641	2
Fagron	Estradiol hemihydrate	18F18-B01-359015	2
Fagron	Estradiol hemihydrate	18F18B01360269	1
Fagron	Estradiol hemihydrate	18F18-B01-360269	1
Fagron	Estradiol hemihydrate	18F18-B01-363586	3
Fagron	Estradiol hemihydrate	18F18-B01-363587	2
Fagron	Estradiol hemihydrate	20B07-F02-369198	1
Fagron	Estradiol hemihydrate	20b07-f02-369199	1
Fagron	Estradiol hemihydrate	20B07-F02-369529	1
Fagron	Estradiol hemihydrate	20I18-F03-374511	1
Fagron	Estradiol hemihydrate	20I18-FO3-374511	2
Fagron	Estradiol hemihydrate	20l18-F03-374511	1
Fagron	Estradiol hemihydrate	21E12-F07-378251	2
Fagron	Estradiol hemihydrate	21E12-F07-378252	1
Fagron	Estradiol hemihydrate	21E12-F07-378866	2
Fagron	Estradiol hemihydrate	302446	1
Fagron	Estradiol hemihydrate	83100820	2
Fagron	Estradiol hemihydrate	84201170	1
Fagron	Estradiol hemihydrate	84201560	1
Fagron	Estradiol hemihydrate	9G07N01	1
Fagron	Estradiol hemihydrate	9J27-N05	1
Fagron	Estradiol hemihydrate	F02-3695209	1
Fagron	Estradiol hemihydrate	UN80044	1
Fargon	Estradiol hemihydrate	2B07-369198	1
Fargon	Estradiol hemihydrate	B01-3635806	1
Fargon	Estradiol hemihydrate	f02-3691908	1
Fargron/ Sanacorp	Estradiol hemihydrate	14G24-b04-297402	1
Fiebig	Estradiol hemihydrate	16H04-B01	1
Gatt-Koller	Estradiol hemihydrate	1801604	2
Gehe	Estradiol hemihydrate	15038016	1
Gehe	Estradiol hemihydrate	82404160	1
Henry Lamotte/AHD	Estradiol hemihydrate	18082101	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
La Chandra /Noweda	Estradiol hemihydrate	210301401	1
Noweda	Estradiol hemihydrate	12268008	1
Noweda	Estradiol hemihydrate	15038004	1
Noweda	Estradiol hemihydrate	18F18-B01_351946	1
Noweda	Estradiol hemihydrate	21003879006	1
phönix	Estradiol hemihydrate	13285802	1
Phönix	Estradiol hemihydrate	21003879002	1
phönix	Estradiol hemihydrate	21003879009	3
Phönix	Estradiol hemihydrate	23000120001	1
Röntgen	Estradiol hemihydrate	18082105	1
Röntgen	Estradiol hemihydrate	193089002	1
Sanacorp /Fargron	Estradiol hemihydrate	15D01-B02-312068	1
Sanacorp	Estradiol hemihydrate	15038010	1
Sanacorp	Estradiol hemihydrate	18F18-B01	1
Sanacorp	Estradiol hemihydrate	21E12-F07-379952	2
Symbiotec/Phoenix	Estradiol hemihydrate	20/18-F03	1
vDL	Estradiol hemihydrate	2103014-02	1

- 235 470 spectra from 1515 *Apo-Ident* customers from a total of 49 094 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Estradiol hemihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Estradiol hemihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	1009	0	151 953
Type B	0	2464	0	199 620
Type C	0	596	1	235 470

The substance/substance group *Estradiol hemihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.4054 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.7565 %)
Type C	100.0000 % (> 99.9007 %)	99.8325 % (> 99.3300 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21291	21945	4.81	107.01
21302	21302	0.00	122.09
21499	21847	6.45	102.43
21500	21500	0.00	96.67
21501	21302	5.59	117.90
21502	21302	5.71	116.43
21503	21302	10.98	116.31
21504	21302	6.78	117.31
21505	21302	9.73	116.01
21506	21945	9.63	110.18
21507	21302	5.80	120.88
21508	21508	0.00	126.71
21667	21945	2.93	108.78
21847	21847	0.00	102.68
21945	21945	0.00	111.18
22307	22307	0.00	114.66
22913	22913	0.00	115.65
23184	22307	4.15	118.79
25402	25402	0.00	116.96
25608	25608	0.00	113.33

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Estradiol valerate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20330-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Estradiol valerate; Estradioli valeras

Special notes

When selecting the *Estradiol valerate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Estradiol valerate	6	4	137

Second-stage model

For differentiation of the substance/substance group *Estradiol valerate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Estradiol valerate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	90.34	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Estradiol valerate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Estradiol valerate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Estradiol valerate	13264001	21411	60	1410503
Caelo	Estradiol valerate	13264001	21411SI	45	1410503
Caelo	Estradiol valerate	13264001	21416	120	1510624
Caelo	Estradiol valerate	13264001	21416SI	45	1510624
Caelo	Estradiol valerate	13264001	21417	20	20130920
Caelo	Estradiol valerate	13264001	21418	20	20130920
Caelo	Estradiol valerate	13264001	21419	20	20130920
Caelo	Estradiol valerate	13264001	21422	20	20130920
Caelo	Estradiol valerate	13264001	21423	20	20130920
Caelo	Estradiol valerate	13264001	21424	60	1410503
Caelo	Estradiol valerate	13264001	21425	20	20130920
Caelo	Estradiol valerate	13264001	21426	20	20130920
Caelo	Estradiol valerate	15194802	21989	60	20150708
Caelo	Estradiol valerate	15194802	21989SI	30	20150708
Caelo	Estradiol valerate	163277	23056	40	20161221*
Caelo	Estradiol valerate	163277	23056SI	40	20161221*
Caelo	Estradiol valerate	22000384013	26741	40	20220407
Fagron	Estradiol valerate	12D18-N02	20651	40	20120426
Fagron	Estradiol valerate	12D18-N02	21266	40	20120118
Fagron	Estradiol valerate	14E26-B02-294846	21646	60	20140616

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 820 spectra of 20 reference samples from the substance/substance group *Estradiol valerate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 142 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 467 spectra of 16 reference samples from the substance/substance group *Estradiol valerate*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Estradiol valerate	180674	24030	40
Caelo	Estradiol valerate	20002389004	25427	40
Caelo	Estradiol valerate	24000954	27231	40
Fagron	Estradiol valerate	20J16-F01-375199	25753	40
Caelo	Estradiol valerate	13264001	21417SI†	14
Caelo	Estradiol valerate	13264001	21418SI†	15
Caelo	Estradiol valerate	13264001	21419SI†	15
Caelo	Estradiol valerate	13264001	21422SI†	17
Caelo	Estradiol valerate	13264001	21423SI†	15
Caelo	Estradiol valerate	13264001	21425SI†	15
Caelo	Estradiol valerate	13264001	21426SI†	16
Caelo	Estradiol valerate	180674	24030SI	40
Caelo	Estradiol valerate	20002389004	25427SI	40
Caelo	Estradiol valerate	22000384013	26741SI†	40
Caelo	Estradiol valerate	24000954	27231SI	40
Fagron	Estradiol valerate	20J16-F01-375199	25753SI	40

- 201 617 spectra from a total of 4039 batches from further 838 substances. These spectra were

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 500 spectra from 207 *Apo-Ident* customers from 147 batches from the substance/substance group *Estradiol valerate*.
- Among them are spectra of independent samples from 137 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Estradiol valerate	22000384002	1
	Estradiol valerate	22000384007	1
	Estradiol valerate	22000384010	2
	Estradiol valerate	22000384011	3
	Estradiol valerate	22000384015	4
	Estradiol valerate	22000384017	2
	Estradiol valerate	22000384021	1
	Estradiol valerate	ESV003-1A	1
	Estradiol valerate	F01-3760807	1
Bayer Pharma / Gehe	Estradiol valerate	84404140	1
Bayer Pharma AG	Estradiol valerate	15C10-B05-305395	1
Bayer Pharma GmbH	Estradiol valerate	82201620	1
Beiersdorf/AHD	Estradiol valerate	12A20-N10	1
Caelo	Estradiol valerate	10E07-N04	1
Caelo	Estradiol valerate	12G05-N09	2
Caelo	Estradiol valerate	13264001	1
Caelo	Estradiol valerate	13264002	1
Caelo	Estradiol valerate	13264003	1
Caelo	Estradiol valerate	14E26-B02-294844	1
Caelo	Estradiol valerate	14E26-B02-294845	1
Caelo	Estradiol valerate	15194808	1
Caelo	Estradiol valerate	15C10-805	1
Caelo	Estradiol valerate	15C10-B05	2
Caelo	Estradiol valerate	15c10-B05-305396	1
Caelo	Estradiol valerate	15C10B05308851	1
Caelo	Estradiol valerate	15c10-b05-314840	1
Caelo	Estradiol valerate	15C10-B05-314840	1
Caelo	Estradiol valerate	15C10-B05-321675	1
Caelo	Estradiol valerate	15C10-B05-326087	1
Caelo	Estradiol valerate	16327702	5
Caelo	Estradiol valerate	16327703	2
Caelo	Estradiol valerate	16327706	4
Caelo	Estradiol valerate	16327709	5
Caelo	Estradiol valerate	16327710	1
Caelo	Estradiol valerate	16327711	3
Caelo	Estradiol valerate	16F09-B01-332756	1
Caelo	Estradiol valerate	18062402	1
Caelo	Estradiol valerate	18067402	11
Caelo	Estradiol valerate	18067403	1
Caelo	Estradiol valerate	18067404	1
Caelo	Estradiol valerate	18067405	2

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Estradiol valerate	18067407	8
Caelo	Estradiol valerate	18067408	2
Caelo	Estradiol valerate	18067409	7
Caelo	Estradiol valerate	18067410	1
Caelo	Estradiol valerate	18067410P-181228-1	1
Caelo	Estradiol valerate	18067411	1
Caelo	Estradiol valerate	18067412	3
Caelo	Estradiol valerate	18067413	2
Caelo	Estradiol valerate	18067415P-190718-2	1
Caelo	Estradiol valerate	18067416	6
Caelo	Estradiol valerate	18067417	1
Caelo	Estradiol valerate	18067417P-200217-3	1
Caelo	Estradiol valerate	1810013	1
Caelo	Estradiol valerate	190615001	4
Caelo	Estradiol valerate	190615003	1
Caelo	Estradiol valerate	190615004	13
Caelo	Estradiol valerate	190615007	3
Caelo	Estradiol valerate	19061501	2
Caelo	Estradiol valerate	19061503	4
Caelo	Estradiol valerate	19061506	5
Caelo	Estradiol valerate	19061507	10
Caelo	Estradiol valerate	200004423006	1
Caelo	Estradiol valerate	20002389002	19
Caelo	Estradiol valerate	20002389003	11
Caelo	Estradiol valerate	20004423001	12
Caelo	Estradiol valerate	20004423003	5
Caelo	Estradiol valerate	20004423005	3
Caelo	Estradiol valerate	20004423006	9
Caelo	Estradiol valerate	2000443001	1
Caelo	Estradiol valerate	2002389002	1
Caelo	Estradiol valerate	218U-03259	1
Caelo	Estradiol valerate	22000384004	2
Caelo	Estradiol valerate	22000384007	1
Caelo	Estradiol valerate	4(20002389002)	1
Caelo	Estradiol valerate	4214U-03259	1
Caelo	Estradiol valerate	5218Q-03259	1
Caelo	Estradiol valerate	5315A-03259	1
Caelo	Estradiol valerate	test	1
Caesar & Lorenz	Estradiol valerate	10123258	1
Caesar & Loretz GmbH...	Estradiol valerate	20004423003	1
Caesar & Loretz GmbH...	Estradiol valerate	20004423006	1
Caesar & Loretz GmbH...	Estradiol valerate	22000384004	1
Caesar & Loretz GmbH...	Estradiol valerate	20004423005	1
Caesar & Loretz GmbH/Gehe	Estradiol valerate	190615	1
Caesar & Loretz GmbH/Gehe	Estradiol valerate	190615004	1
Caesar & Loretz GmbH/Kehr	Estradiol valerate	18067409	1
Caesar & Loretz GmbH/Kehr	Estradiol valerate	18067416	1
Caesar & Loretz GmbH...	Estradiol valerate	20004423005	1
Caesar & Loretz GmbH...	Estradiol valerate	19061501	1
Caesar & Loretz GmbH...	Estradiol valerate	19061507	4
Caesar & Loretz GmbH...	Estradiol valerate	20004423006	3
Caesar & Loretz GmbH...	Estradiol valerate	20002389002	1
Caesar & Loretz GmbH	Estradiol valerate	18067416	1
Caesar & Loretz GmbH	Estradiol valerate	18067417	1
CAESAR & LORETZ GMBH	Estradiol valerate	190615001	1
CAESAR & LORETZ GMBH	Estradiol valerate	190615003	2
Caesar & Loretz GmbH	Estradiol valerate	190615004	4
Caesar & Loretz GmbH	Estradiol valerate	19061503	2
Caesar & Loretz GmbH	Estradiol valerate	19061507	1
Caesar & Loretz GmbH	Estradiol valerate	20002389002	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Estradiol valerate	20002389003	2
Caesar & Loretz GmbH	Estradiol valerate	20004423001	5
Caesar & Loretz GmbH	Estradiol valerate	20004423003	3
Caesar & Loretz GmbH	Estradiol valerate	20004423006	7
Caesar & Loretz GmbH	Estradiol valerate	22000384002	4
Caesar & Loretz GmbH	Estradiol valerate	22000384004	4
Caesar & Loretz GmbH	Estradiol valerate	22000384005	1
Cealo/Sanacorp	Estradiol valerate	20004423006	1
Euro OTC	Estradiol valerate	15C10-b05	1
Euro OTC	Estradiol valerate	1606022-01	1
Faegon	Estradiol valerate	15C10-B05-324956	2
Fagro	Estradiol valerate	15C10-B05-318405	1
Fagron	Estradiol valerate	11G18-N04	1
Fagron	Estradiol valerate	11J13-N09	1
Fagron	Estradiol valerate	11J13-No9	1
Fagron	Estradiol valerate	11k04-n04	1
Fagron	Estradiol valerate	11K04-N04	1
Fagron	Estradiol valerate	12A20-N10	2
Fagron	Estradiol valerate	12D18-N02	3
Fagron	Estradiol valerate	12G05N09	1
Fagron	Estradiol valerate	12G05-N09	2
Fagron	Estradiol valerate	12K05-N02	3
Fagron	Estradiol valerate	13A07-N11	6
Fagron	Estradiol valerate	13D16N10	1
Fagron	Estradiol valerate	13D16-N10	4
Fagron	Estradiol valerate	13g09-n05	1
Fagron	Estradiol valerate	13G09N05	1
Fagron	Estradiol valerate	13G09-N05	5
Fagron	Estradiol valerate	13I13-N02	2
Fagron	Estradiol valerate	13J13-N02	1
Fagron	Estradiol valerate	14E26B02	2
Fagron	Estradiol valerate	14E26-B02-294844	1
Fagron	Estradiol valerate	14E26-B02-294845	3
Fagron	Estradiol valerate	14E26-B02-294847	1
Fagron	Estradiol valerate	14E26-B02-296348	7
Fagron	Estradiol valerate	14E26-B02-302873	3
Fagron	Estradiol valerate	15C10-B05	2
Fagron	Estradiol valerate	15C10-B05_314840	1
Fagron	Estradiol valerate	15C10-B05-305395	6
Fagron	Estradiol valerate	15C10-B05-305396	1
Fagron	Estradiol valerate	15C10-B05-308851	9
Fagron	Estradiol valerate	15c10-b05-309186	1
Fagron	Estradiol valerate	15C10-B05-309186	3
Fagron	Estradiol valerate	15C10-B05-313568	1
Fagron	Estradiol valerate	15c10-b05-314840	1
Fagron	Estradiol valerate	15C10-B05-314840	5
Fagron	Estradiol valerate	15C10-B05-318405	1
Fagron	Estradiol valerate	15C10B05321675	1
Fagron	Estradiol valerate	15C10-B05-321675	11
Fagron	Estradiol valerate	15c10-b05-324956	1
Fagron	Estradiol valerate	15C10-B05-324956	1
Fagron	Estradiol valerate	15C10B05-326087	1
Fagron	Estradiol valerate	15C10-B05-326087	5
Fagron	Estradiol valerate	16F09-B01	2
Fagron	Estradiol valerate	16F09-B01_332756	1
Fagron	Estradiol valerate	16F09-B01-328135	8
Fagron	Estradiol valerate	16F09-B01-329621	1
Fagron	Estradiol valerate	16F09-B01-332756	7
Fagron	Estradiol valerate	16F09-B01-332757	2
Fagron	Estradiol valerate	16F09Bo1328135	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Estradiol valerate	18067405	1
Fagron	Estradiol valerate	18g05-b02	1
Fagron	Estradiol valerate	18G05-B02	2
Fagron	Estradiol valerate	18G05-B02-353985	13
Fagron	Estradiol valerate	18G05-B02353986	1
Fagron	Estradiol valerate	18G05-B02-353986	3
Fagron	Estradiol valerate	18G5-B02-253985	1
Fagron	Estradiol valerate	190615001	1
Fagron	Estradiol valerate	19c10-b05-318405	1
Fagron	Estradiol valerate	20002389003	1
Fagron	Estradiol valerate	20J16-F01	2
Fagron	Estradiol valerate	20J16-F01-3760807	1
Fagron	Estradiol valerate	20J16F01376087	2
Fagron	Estradiol valerate	20J16-F01-376087	3
Fagron	Estradiol valerate	23A30-B05-224547	1
Fagron	Estradiol valerate	24052014a	1
Fagron	Estradiol valerate	27061710	1
Fagron	Estradiol valerate	814M-03259	1
Fagron	Estradiol valerate	82201620	1
Fagron	Estradiol valerate	84404140	4
Fagron	Estradiol valerate	ESV003-1A	2
Fagron	Estradiol valerate	ESVOO3-1A	1
Fagron	Estradiol valerate	F01-3751904	1
Fagron	Estradiol valerate	VFM002-1C	2
Fargon / AHD	Estradiol valerate	18G05-B02-353985	2
Fargon	Estradiol valerate	10123264	1
Frago/Gehe	Estradiol valerate	15C10-B0508561040	1
Frago/Noweda	Estradiol valerate	16F09-B01	2
Frago/Noweda	Estradiol valerate	16F09-B01-329621	1
Frago/Noweda	Estradiol valerate	16F09-B01-332757	1
Fragon	Estradiol valerate	15C10-B05-5314840	1
Gehe	Estradiol valerate	14E26-B02-296348	1
Gehe	Estradiol valerate	14E26-B02-302872	1
Gehe	Estradiol valerate	16327703	1
Gehe	Estradiol valerate	16327712	1
Gehe	Estradiol valerate	16F09-B01-332756	1
GEHE	Estradiol valerate	16F09-B01-332757	1
Gehe	Estradiol valerate	190615001	1
Hedinger/Noweda	Estradiol valerate	15C10-B05	1
Noweda	Estradiol valerate	12A20-N10	1
Noweda	Estradiol valerate	19061506	1
Noweda	Estradiol valerate	20002389003	1
noweda	Estradiol valerate	2200034007	1
Noweda	Estradiol valerate	22000384015	1
Phoenix	Estradiol valerate	13G09-N05	1
Phoenix	Estradiol valerate	20002389002	1
Phoenix	Estradiol valerate	20J16-F01-375194	1
Phönix/Fargon	Estradiol valerate	979-32-8	1
Phönix	Estradiol valerate	15C10-B05-326087	1
phönix	Estradiol valerate	20J16-F01	1
Röntgen	Estradiol valerate	190615004	2
Sanacorp	Estradiol valerate	13264002	1
Sanacorp	Estradiol valerate	20J16-F01-375194	1
Sanacorp	Estradiol valerate	22000384015	1
THC/Phönix	Estradiol valerate	18067402	1

- 235 567 spectra from 1515 *Apo-Ident* customers from a total of 49 113 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Estradiol valerate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Estradiol valerate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	820	0	152 142
Type B	0	467	0	201 617
Type C	0	492	8	235 567

The substance/substance group *Estradiol valerate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.2683 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.7152 %)
Type C	100.0000 % (> 99.9007 %)	98.4000 % (> 97.8000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20651	21411	5.63	126.35
21266	21416	6.29	128.75
21411	21411	0.00	125.50
21416	21416	0.00	128.51
21417	21416	2.65	129.03
21418	21416	4.99	126.77
21419	21416	1.87	128.95
21422	21416	3.72	129.47
21423	21416	3.00	127.83
21424	21424	0.00	128.94
21425	21416	2.39	129.60
21426	21416	1.88	129.03
21646	21416	5.49	129.26

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21989	21416	2.72	129.89
23056	23056	0.00	128.64
26741	21416	10.35	127.44

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Estriol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20878-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Estriol; Estriolum

Special notes

When selecting the *Estriol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Estriol	8	19	195

Second-stage model

For differentiation of the substance/substance group *Estriol* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Estriol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	59.24	–
⋮	⋮	⋮
Polymyxin B sulfate	>50	36.89
Bacitracin	>50	55.12
Estradiol hemihydrate	>50	55.51
Riboflavin	>50	79.05
Colistin sulfate	>50	79.33
Amphotericin B	>50	85.38
Cyanocobalamin	>50	120.17
Triamcinolone	>50	128.67
Calcium pantothenate	>50	135.64
Nystatin	>50	148.75
alpha-tocopheryl acetate dry concentrate	>50	176.15
Selenium yeast	>50	201.07
Tosylchloramide sodium	>50	203.77
Hyoscine hydrobromide	>50	222.98
Methylcobalamin	>50	226.25
Calcium glycerophosphate	>50	237.35
Gelatine, white	>50	264.73
Carmellose sodium	>50	342.14
SyrSpend® SF pH4 neo (Maize starch)	>50	413.17
SyrSpend® SF Alka	>50	416.35
Oxalic acid	>50	420.81
Rice starch	>50	554.85
Corn starch	>50	634.93
Wheat starch	>50	662.17
Acacia, dried dispersion	>50	665.64
Maltodextrin	>50	862.70
SyrSpend® SF pH4	>50	888.58
Potato starch	>50	919.78
Fructose	>50	1031.11

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Estriol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

substance/substance group *Estriol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Estriol	12298706	20878	40	20121106
Caelo	Estriol	13256001	21390	55	1511155
Caelo	Estriol	13256001	21390SI	60	1511155
Caelo	Estriol	13256001	21391	60	20130821
Caelo	Estriol	13256001	21392	20	20130821
Caelo	Estriol	13256001	21393	60	20130821
Caelo	Estriol	13256001	21394	20	20130821
Caelo	Estriol	13256001	21395	20	20130821
Caelo	Estriol	13256001	21399	20	20130821
Caelo	Estriol	13256001	21400	20	20130821
Caelo	Estriol	13256001	21401	20	20130821
Caelo	Estriol	13256001	21404	20	20130821
Euro OTC	Estriol	1507026	21848	60	0000010671
Euro OTC	Estriol	1507026	21848SI	60	0000010671
Euro OTC	Estriol	1509042	21939	60	20151009*
Euro OTC	Estriol	1509042	21939SI	60	20151009*
Euro OTC	Estriol	1703044	23181	40	20170502*
Fagron	Estriol	11J13-N07	21255	40	1412180
Fagron	Estriol	16D15-B03-322957	22889	40	20160711
Fagron	Estriol	16D15-B03-322957	22889SI	40	20160711
Fagron	Estriol	16I19-B01-331468	23172	40	20170301

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 855 spectra of 21 reference samples from the substance/substance group *Estriol*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.
- 152 107 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 1777 spectra of 47 reference samples from the substance/substance group *Estriol*.
- Among them are spectra of independent samples from 19 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Estriol	161382	22633	40
Caelo	Estriol	2010002	25400	40
Caelo	Estriol	22003580	26715	39
Euro OTC	Estriol	1310002-01	21292	40
Euro OTC	Estriol	1606044	22711	40
Euro OTC	Estriol	1610035	22850	40
Euro OTC	Estriol	1710022	23731	40
Euro OTC	Estriol	1710030	23733	40
Euro OTC	Estriol	1803011	24073	40
Euro OTC	Estriol	1903035	24604	40
Euro OTC	Estriol	2002010	25107	40
Euro OTC	Estriol	2007001	25237	40
Euro OTC	Estriol	2103007	25610	40
Euro OTC	Estriol	2107006	25706	50
Euro OTC	Estriol	2111005	25884	50
Euro OTC	Estriol	2302018	26660	40
Euro OTC	Estriol	2312004	27158	39
Euro OTC	Estriol	2402025	27286	40
Fagron	Estriol	22H12-B05-224456	26455	40
Caelo	Estriol	13256001	21391SI†	60
Caelo	Estriol	13256001	21392SI†	20
Caelo	Estriol	13256001	21394SI†	20
Caelo	Estriol	13256001	21395SI†	20
Caelo	Estriol	13256001	21399SI†	20
Caelo	Estriol	13256001	21400SI†	20
Caelo	Estriol	13256001	21401SI†	20
Caelo	Estriol	13256001	21404SI†	20
Caelo	Estriol	161382	22633SI	40
Caelo	Estriol	2010002	25400SI	40
Caelo	Estriol	22003580	26715SI	40
Euro OTC	Estriol	1606044	22711SI	40
Euro OTC	Estriol	1610035	22850SI	40
Euro OTC	Estriol	1703044	23181SI†	40
Euro OTC	Estriol	1710022	23731SI	40
Euro OTC	Estriol	1710030	23733SI	40
Euro OTC	Estriol	1803011	24073SI	40
Euro OTC	Estriol	1903035	24604SI	40
Euro OTC	Estriol	2002010	25107SI	40
Euro OTC	Estriol	2007001	25237SI	40
Euro OTC	Estriol	2103007	25610SI	40
Euro OTC	Estriol	2107006	25706SI	50
Euro OTC	Estriol	2111005	25884SI	50
Euro OTC	Estriol	2302018	26660SI	40
Euro OTC	Estriol	2312004	27158SI	30
Euro OTC	Estriol	2402025	27286SI	40
Fagron	Estriol	16I19-B01-331468	23172SI†	30
Fagron	Estriol	22H12-B05-224456	26455SI	39

- 200 307 spectra from a total of 4023 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 628 spectra from 300 *Apo-Ident* customers from 203 batches from the substance/substance group *Estriol*.
- Among them are spectra of independent samples from 185 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Estriol	20G10-f06-372935	1
	Estriol	20G10-F06-372935	1
	Estriol	21002272024	1
	Estriol	22003680002	1
	Estriol	22H12-B06-222366	2
	Estriol	23A30-B01-227260	1
	Estriol	23A30-B01-227261	1
	Estriol	B06-2223606	1
	Estriol	L00048288	1
AHD	Estriol	16I19-B01-331466	1
apomix	Estriol	14077904	1
Apotheke am Luisenho...	Estriol	20000085004	2
Audor Pharma	Estriol		16
Audor Pharma	Estriol	2002010-01	1
Audor Pharma	Estriol	AP20780041010218E	1
Audor Pharma	Estriol	AP20780041020218E	3
Audor Pharma	Estriol	APL000036940E	1
Audor Pharma	Estriol	APL00036940E	2
Audor Pharma	Estriol	APL00037293	1
Audor Pharma	Estriol	APL00037293E	1
Aufor/AHD	Estriol		1
Bayer Pharma GmbH / ...	Estriol	15297804	1
Bombastus	Estriol	5128	1
Caelo	Estriol	10053206	1
Caelo	Estriol	10H30-N06	1
Caelo	Estriol	11254402	1
Caelo	Estriol	11254410	1
Caelo	Estriol	11254412	1
Caelo	Estriol	12032503	4
Caelo	Estriol	12032504	2
Caelo	Estriol	12032507	5
Caelo	Estriol	12298702	2
Caelo	Estriol	12298704	6
Caelo	Estriol	12298706	1
Caelo	Estriol	12298707	2
Caelo	Estriol	12H06N02	1
Caelo	Estriol	12H06-N02	1
Caelo	Estriol	13256001	1
Caelo	Estriol	13256004	9
Caelo	Estriol	14077901	1
Caelo	Estriol	14077903	2
Caelo	Estriol	14077904	9
Caelo	Estriol	1409018-01	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Estriol	14272101	3
Caelo	Estriol	14272104	5
Caelo	Estriol	1477904	1
Caelo	Estriol	14j20-b07	1
Caelo	Estriol	15008902	1
Caelo	Estriol	15028901	4
Caelo	Estriol	15028904	8
Caelo	Estriol	15028905	1
Caelo	Estriol	15297804	17
Caelo	Estriol	15297805	1
Caelo	Estriol	16/19-B01-331467	1
Caelo	Estriol	16053404	1
Caelo	Estriol	16053405	2
Caelo	Estriol	16053408	5
Caelo	Estriol	16053409	1
Caelo	Estriol	16138204	4
Caelo	Estriol	16317701	5
Caelo	Estriol	16317702	6
Caelo	Estriol	16317703	4
Caelo	Estriol	17042014B	1
Caelo	Estriol	1710030-01	2
Caelo	Estriol	17133703	2
Caelo	Estriol	17133704	9
Caelo	Estriol	17133705	4
Caelo	Estriol	17133706	21
Caelo	Estriol	17133709	6
Caelo	Estriol	17133710	8
Caelo	Estriol	17133711	6
Caelo	Estriol	1713373	1
Caelo	Estriol	1733706	1
Caelo	Estriol	17348701	17
Caelo	Estriol	17348702	9
Caelo	Estriol	17348706	10
Caelo	Estriol	17348707	8
Caelo	Estriol	18041811	1
Caelo	Estriol	18247101	4
Caelo	Estriol	19035606	3
Caelo	Estriol	19035607	10
Caelo	Estriol	19035609	2
Caelo	Estriol	200000085004	1
Caelo	Estriol	20000085004	18
Caelo	Estriol	20000085005	1
Caelo	Estriol	20000085006	6
Caelo	Estriol	20G10-F06	1
Caelo	Estriol	20G10-F06-372934	1
Caelo	Estriol	20G10-F06-372958	1
Caelo	Estriol	24031501	1
Caelo	Estriol	27061303	1
Caelo	Estriol	9071801	1
Caelo	Estriol	L00047276	1
Caesar & Loretz GmbH...	Estriol	20000085004	1
Caesar & Loretz GmbH...	Estriol	20000085006	1
Caesar & Loretz GmbH...	Estriol	19035607	1
Caesar & Loretz GmbH...	Estriol	20000085006	1
Caesar & Loretz GmbH...	Estriol	20000085006	1
Caesar & Loretz GmbH	Estriol	15028901	1
Caesar & Loretz GmbH	Estriol	15028904	1
Caesar & Loretz GmbH	Estriol	17133704	1
Caesar & Loretz GmbH	Estriol	17348701	1
Caesar & Loretz GmbH	Estriol	19035607	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Estriol	19035609	2
Caesar & Loretz GmbH	Estriol	20000085004	2
Caesar & Loretz GmbH	Estriol	20000085006	2
Caesar & Loretz GmbH	Estriol	21001836002	1
Caesar § Lorenz GmbH	Estriol	12298712	1
Caesar&Loretz,AHC, 1...	Estriol	15297804	1
Cealo/ Sanacorp	Estriol	17133706	2
Cealo/GEHE	Estriol	17348702	1
Ensbona/ Sanacorp	Estriol	16053405	1
EuRho	Estriol	1710030-01	1
Euro OTC	Estriol	1201020-01	1
Euro OTC	Estriol	1310002-01	1
Euro OTC	Estriol	1403011-01	2
Euro OTC	Estriol	1409018-01	1
Euro OTC	Estriol	15028904	1
Euro OTC	Estriol	1507026-01	1
Euro OTC	Estriol	1509042-01	3
Euro OTC	Estriol	1606044-01	14
Euro OTC	Estriol	1610035-01	5
Euro OTC	Estriol	1703044-01	1
Euro OTC	Estriol	170344-01	1
Euro OTC	Estriol	1710030-01	3
Euro OTC	Estriol	17133706	1
Euro OTC	Estriol	1803011-01	1
Euro OTC	Estriol	1903035-01	1
Euro OTC	Estriol	2002010-01	1
Euro OTC	Estriol	2007001-01	6
Euro OTC	Estriol	2010002-01	4
Euro OTC	Estriol	2010002-03	3
Euro OTC	Estriol	2103007-01	7
Euro OTC	Estriol	2107006-01	2
Euro/Phönix	Estriol	1509042-01	1
Fagron	Estriol		2
Fagron	Estriol	11D13-N11	1
Fagron	Estriol	11J13-N07	3
Fagron	Estriol	12A26-N02	2
Fagron	Estriol	12F08-N06	1
Fagron	Estriol	12H06-N02	5
Fagron	Estriol	12H06-No2	2
Fagron	Estriol	12K07-N15	2
Fagron	Estriol	13C15-N04	4
Fagron	Estriol	13D19-N02	1
Fagron	Estriol	13H28-N01	4
Fagron	Estriol	14B06-B11-291563	1
Fagron	Estriol	14b06b11291565	1
Fagron	Estriol	14B06-B11-291565	1
Fagron	Estriol	14B06-B11-294565	1
Fagron	Estriol	14E13-B01-294033	1
Fagron	Estriol	14E13-B01-294034	3
Fagron	Estriol	15297804	2
Fagron	Estriol	15A15-B07-312064	2
Fagron	Estriol	15A15-B07-314241	2
Fagron	Estriol	16/19-B01-332862	1
Fagron	Estriol	16/19-B01-336394	1
Fagron	Estriol	16/19-B01-340536	3
Fagron	Estriol	16/19-B01-3430535	1
Fagron	Estriol	16/19-B01-348555	1
Fagron	Estriol	16/19-B01-351346	3
Fagron	Estriol	1619B01351346	1
Fagron	Estriol	1629-b01-3363964	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Estriol	16D15-B03-323016	2
Fagron	Estriol	16D15-B03-323017	1
Fagron	Estriol	16I19-B01	2
Fagron	Estriol	16I19-B01-331466	1
Fagron	Estriol	16I19-B01-331467	1
Fagron	Estriol	16I19-B01-331468	1
Fagron	Estriol	16I19-B01-332862	1
Fagron	Estriol	16I19-B01-340535	2
Fagron	Estriol	16I19-B01-348555	1
Fagron	Estriol	16I19-B01-351346	1
Fagron	Estriol	16I9-B01	1
Fagron	Estriol	19C28-B01	1
Fagron	Estriol	19C28-B01-361787	3
Fagron	Estriol	19C28-B01-361788	1
Fagron	Estriol	20F16-F02	1
Fagron	Estriol	20F16-F02-372831	1
Fagron	Estriol	20f16-f02-372833	1
Fagron	Estriol	20G10-F06	7
Fagron	Estriol	20G10-F06-3729304	1
Fagron	Estriol	20G10-F06-372933	1
Fagron	Estriol	20g10-f06-372934	1
Fagron	Estriol	20g10-F06-372934	1
Fagron	Estriol	20G10-F06-372934	15
Fagron	Estriol	20G10-F06-372936	1
Fagron	Estriol	20G10-F06372958	1
Fagron	Estriol	20G10-F06-372958	28
Fagron	Estriol	20G10-F06-379234	1
Fagron	Estriol	20G10-FO6-372935	1
Fagron	Estriol	20G10-FO6-372958	1
Fagron	Estriol	21B26-F01	1
Fagron	Estriol	21B26-F01-378475	1
Fagron	Estriol	21B26-F01-379597	1
Fagron	Estriol	21B26-F01-380778	1
Fagron	Estriol	22A10-F03-381434	2
Fagron	Estriol	22A10-F03-381730	1
Fagron	Estriol	22H12-B05-224456	1
Fagron	Estriol	22H12-B06	1
Fagron	Estriol	22H12-B06-222365	3
Fagron	Estriol	22H12-B06-222366	1
Fagron	Estriol	22H12-BO6-222366	1
Fagron	Estriol	23A30-B01-227262	1
Fagron	Estriol	23H03-B06-233745	1
Fagron	Estriol	2OG10-F06-372934	1
Fagron	Estriol	2OG10-FO6-372934	1
Fagron	Estriol	700194-0001	1
Fagron	Estriol	81100490	1
Fagron	Estriol	86200800	3
Fagron	Estriol	F02-3728302	1
Fagron	Estriol	F06_3729508	1
Fagron	Estriol	F06-3729303	1
Fagron	Estriol	F06-3729304	3
Fagron	Estriol	F06-372933	1
Fagron	Estriol	F06-3729508	3
Fagron	Estriol	L00047276	11
fargon	Estriol	12a26-n02	1
Fiebig	Estriol	17133711	2
Fischar/Gehe	Estriol	14H29-B02-298072	3
Gehe 30.12.14	Estriol	14B06-B11-291563	1
Gehe	Estriol	16053405	1
Gehe	Estriol	17348701	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Geilenkirchen	Estriol	17133706	1
Geilenkirchen	Estriol	17133710	1
Geilenkirchen	Estriol	17348701	1
Haihang Industry	Estriol	20130824	1
Jenne	Estriol	F06-3729508	1
Kehr	Estriol	17133704	1
Kehr	Estriol	18247101	1
Noweda 19.05.2015	Estriol	14272104	1
Noweda	Estriol	11J13-No7	1
Noweda	Estriol	12032504	1
Noweda	Estriol	16I19-B01	1
Noweda	Estriol	19C28-B01-361786	1
Noweda	Estriol	20G10-F06	1
Noweda	Estriol	20G10-F06-372933	2
Noweda	Estriol	2103007	1
NWM CHina	Estriol	ES150304	1
Phoenix	Estriol	17348701	1
Phoenix	Estriol	20G10-F06-372958	1
Phoenix	Estriol	3032	1
Phönix /euro	Estriol	1803011-01	1
Phönix	Estriol	16/19-B01331467	1
Sanacorp	Estriol	13256004	1
Sanacorp	Estriol	16317701	1
Sanacorp	Estriol	16317702	1
Sanacorp	Estriol	19035606	1
sanacorp	Estriol	2103007-01	1
Sanacorp	Estriol	2111005-01	1
Shandong Northwest M…	Estriol	ETL160302	1
Shandong Northwest M…	Estriol	ETL160419	1
VDL	Estriol	13256004	1

- 235 439 spectra from 1515 *Apo-Ident* customers from a total of 49 058 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Estriol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Estriol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	855	0	152 107
Type B	0	1777	0	200 307
Type C	0	618	10	235 439

The substance/substance group *Estriol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.2982 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.6624 %)
Type C	100.0000 % (> 99.9007 %)	98.4076 % (> 97.9299 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20878	21255	5.90	179.06
21255	21255	0.00	177.90
21390	21390	0.00	196.83
21391	21390	5.03	197.39
21392	21939	5.34	194.64
21393	21848	5.67	196.31
21394	21939	4.82	193.04
21395	21848	2.43	198.69
21399	21939	2.91	174.98
21400	21939	4.60	178.71
21401	21390	3.59	199.38
21404	21939	3.20	168.17
21848	21848	0.00	198.84
21939	21939	0.00	178.08
22889	23181	3.03	150.27
23172	21939	3.78	159.36
23181	23181	0.00	152.73

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ethacridine lactate monohydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20750-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ethacridine lactate monohydrate; Ethacridini lactas monohydricus

Special notes

When selecting the *Ethacridine lactate monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ethacridine lactate monohydrate	7	5	94

Second-stage model

For differentiation of the substance/substance group *Ethacridine lactate monohydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ethacridine lactate monohydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	76.59	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ethacridine lactate monohydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ethacridine lactate monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ethacridine lactate monoh…	12149507	20750	40	20120619
Caelo	Ethacridine lactate monoh…	16273403	23247	40	20161122
Caelo	Ethacridine lactate monoh…	22001737	26357	40	20220819*
Euro OTC	Ethacridine lactate monoh…	1206016-02	21636	60	20121019
Euro OTC	Ethacridine lactate monoh…	1412034-02	22733	40	20150223
Fagron	Ethacridine lactate monoh…	13I24-N03	21265	40	AR-15-FG-007011-02
Fagron	Ethacridine lactate monoh…	15A29-B02-306219	22500	40	20150205

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 300 spectra of 7 reference samples from the substance/substance group *Ethacridine lactate monohydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 662 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 280 spectra of 9 reference samples from the substance/substance group *Ethacridine lactate monohydrate*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ethacridine lactate monoh…	172476	23671	40
Caelo	Ethacridine lactate monoh…	183146	24355	40
Caelo	Ethacridine lactate monoh…	20001048	25203	40
Caelo	Ethacridine lactate monoh…	21001424012	25925	40
Fagron	Ethacridine lactate monoh…	21C17-B01-215098	26065	40
Caelo	Ethacridine lactate monoh…	172476	23798	40
Caelo	Ethacridine lactate monoh…	21001424012	25925SI	10
Caelo	Ethacridine lactate monoh…	22001737	26357SI†	20
Fagron	Ethacridine lactate monoh…	21C17-B01-215098	26065SI	10

- 201 804 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 451 spectra from 270 *Apo-Ident* customers from 101 batches from the substance/substance group *Ethacridine lactate monohydrate*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 94 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ethacridine lactate monoh...	22001737005	1
	Ethacridine lactate monoh...	22001737011	2
AHD	Ethacridine lactate monoh...	22001737016	1
AHL	Ethacridine lactate monoh...	141101	1
Alliance Healthcare	Ethacridine lactate monoh...	141234-04	1
Anzag	Ethacridine lactate monoh...	111201	1
Anzag	Ethacridine lactate monoh...	18314601	1
Bombastus	Ethacridine lactate monoh...	13/24-N03	1
Bombastus	Ethacridine lactate monoh...	14A15-B04-300493	1
cae	Ethacridine lactate monoh...	16272410	1
cae	Ethacridine lactate monoh...	20004177003	1
Caelo	Ethacridine lactate monoh...	10288702	1
Caelo	Ethacridine lactate monoh...	11J07-N05	1
Caelo	Ethacridine lactate monoh...	1206016-03	1
Caelo	Ethacridine lactate monoh...	12149507	3
Caelo	Ethacridine lactate monoh...	12268407	3
Caelo	Ethacridine lactate monoh...	12G02-N13	2
Caelo	Ethacridine lactate monoh...	141203401	1
Caelo	Ethacridine lactate monoh...	1412034-01	1
Caelo	Ethacridine lactate monoh...	1412034-02	1
Caelo	Ethacridine lactate monoh...	1412034-03	2
Caelo	Ethacridine lactate monoh...	141203404	1
Caelo	Ethacridine lactate monoh...	1412034-04	2
Caelo	Ethacridine lactate monoh...	15/214/R	1
Caelo	Ethacridine lactate monoh...	15177603	4
Caelo	Ethacridine lactate monoh...	15177608	2
Caelo	Ethacridine lactate monoh...	15177612	1
Caelo	Ethacridine lactate monoh...	15438003	6
Caelo	Ethacridine lactate monoh...	15438007	4
Caelo	Ethacridine lactate monoh...	15438009	2
Caelo	Ethacridine lactate monoh...	16272401	1
Caelo	Ethacridine lactate monoh...	16272406	1
Caelo	Ethacridine lactate monoh...	16272408	3
Caelo	Ethacridine lactate monoh...	16272410	3
Caelo	Ethacridine lactate monoh...	16272412	1
Caelo	Ethacridine lactate monoh...	16272413	1
Caelo	Ethacridine lactate monoh...	162734	1
Caelo	Ethacridine lactate monoh...	16273403	8
Caelo	Ethacridine lactate monoh...	16273411	9
Caelo	Ethacridine lactate monoh...	1627412	1
Caelo	Ethacridine lactate monoh...	17247605	14
Caelo	Ethacridine lactate monoh...	17247606	1
Caelo	Ethacridine lactate monoh...	17332303	4
Caelo	Ethacridine lactate monoh...	17332304	16
Caelo	Ethacridine lactate monoh...	17332312	4
Caelo	Ethacridine lactate monoh...	17332314	12
Caelo	Ethacridine lactate monoh...	17332316	6
Caelo	Ethacridine lactate monoh...	1814607	1
Caelo	Ethacridine lactate monoh...	183146004	4
Caelo	Ethacridine lactate monoh...	183146005	6
Caelo	Ethacridine lactate monoh...	18314601	9
Caelo	Ethacridine lactate monoh...	18314603	1
Caelo	Ethacridine lactate monoh...	18314605	1
Caelo	Ethacridine lactate monoh...	18314607	27
Caelo	Ethacridine lactate monoh...	18314608	1
Caelo	Ethacridine lactate monoh...	20001048002	9
Caelo	Ethacridine lactate monoh...	20001048004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ethacridine lactate monoh…	20004177003	10
Caelo	Ethacridine lactate monoh…	21001424004	13
Caelo	Ethacridine lactate monoh…	21001424012	1
Caelo	Ethacridine lactate monoh…	21001424013	1
Caelo	Ethacridine lactate monoh…	21001424014	5
Caelo	Ethacridine lactate monoh…	22001737003	7
Caelo	Ethacridine lactate monoh…	22001737008	1
Caelo	Ethacridine lactate monoh…	22001737011	1
Caelo	Ethacridine lactate monoh…	22001737013	1
Caelo	Ethacridine lactate monoh…	2201737003	1
Caelo	Ethacridine lactate monoh…	7247805	1
Caesar & Lorenz GmbH	Ethacridine lactate monoh…	18314601	1
Caesar & Loretz GmbH…	Ethacridine lactate monoh…	18314601	1
Caesar & Loretz GmbH…	Ethacridine lactate monoh…	17332304	1
Caesar & Loretz GmbH…	Ethacridine lactate monoh…	17332314	1
Caesar & Loretz GmbH…	Ethacridine lactate monoh…	18314601	1
Caesar & Loretz GmbH…	Ethacridine lactate monoh…	20004177003	1
Caesar & Loretz GmbH/AHD	Ethacridine lactate monoh…	20001048002	1
Caesar & Loretz GmbH…	Ethacridine lactate monoh…	22001737003	1
Caesar & Loretz GmbH…	Ethacridine lactate monoh…	17332316	1
Caesar & Loretz GmbH…	Ethacridine lactate monoh…	20001048002	1
Caesar & Loretz GmbH…	Ethacridine lactate monoh…	18314607	1
Caesar & Loretz GmbH/Kehr	Ethacridine lactate monoh…	21001424004	1
Caesar & Loretz GmbH…	Ethacridine lactate monoh…	22001737003	1
Caesar & Loretz GmbH…	Ethacridine lactate monoh…	20001048	1
Caesar & Loretz GmbH	Ethacridine lactate monoh…	17332314	1
Caesar & Loretz GmbH	Ethacridine lactate monoh…	183146002	1
Caesar & Loretz GmbH	Ethacridine lactate monoh…	183146005	3
Caesar & Loretz GmbH	Ethacridine lactate monoh…	18314601	3
Caesar & Loretz GmbH	Ethacridine lactate monoh…	18314607	1
Caesar & Loretz GmbH	Ethacridine lactate monoh…	20001048002	4
Caesar & Loretz GmbH	Ethacridine lactate monoh…	20001048003	1
Caesar & Loretz GmbH	Ethacridine lactate monoh…	20001048006	1
Caesar & Loretz GmbH	Ethacridine lactate monoh…	20004177003	2
Caesar & Loretz GmbH	Ethacridine lactate monoh…	21001424004	2
Caesar & Loretz GmbH	Ethacridine lactate monoh…	21001424012	2
Caesar & Loretz GmbH	Ethacridine lactate monoh…	21001424013	1
Caesar & Loretz GmbH	Ethacridine lactate monoh…	22001737008	1
Caesar & Loretz GmbH	Ethacridine lactate monoh…	caelo	1
Caesar & Loretz/Gehe	Ethacridine lactate monoh…	20001048002	1
Caleo/ Noweda	Ethacridine lactate monoh…	17332312	1
Cealo/Sanacorp	Ethacridine lactate monoh…	21001424013	1
Chinosol/Anzag	Ethacridine lactate monoh…	2112A-02196	1
Chinosol/Anzag	Ethacridine lactate monoh…	914E-02196	1
Dermapharm	Ethacridine lactate monoh…	100201	1
Dermapharm	Ethacridine lactate monoh…	111201	5
Dermapharm	Ethacridine lactate monoh…	130201	8
Dermapharm	Ethacridine lactate monoh…	141101	11
Dermopharm	Ethacridine lactate monoh…	130201	1
Dermopharm	Ethacridine lactate monoh…	141101	1
E Plus	Ethacridine lactate monoh…	17332314	1
Ebert & Jacobi 19…	Ethacridine lactate monoh…	141101	2
Ebert & Jacobi	Ethacridine lactate monoh…	15177608	1
Euro OTC	Ethacridine lactate monoh…	1206016-02	4
Euro OTC	Ethacridine lactate monoh…	1206016-03	6
Euro OTC	Ethacridine lactate monoh…	13/24-N03	1
Euro OTC	Ethacridine lactate monoh…	1412034-01	5
Euro OTC	Ethacridine lactate monoh…	1412034-02	2
Euro OTC	Ethacridine lactate monoh…	1412034-03	13
Euro OTC	Ethacridine lactate monoh…	141203404	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Ethacridine lactate monoh…	1412034-04	4
Euro OTC	Ethacridine lactate monoh…	15438007	1
Euro OTC	Ethacridine lactate monoh…	17332304	2
Euro OTC	Ethacridine lactate monoh…	1807013-01	9
Euro OTC	Ethacridine lactate monoh…	1807013-02	4
Euro OTC	Ethacridine lactate monoh…	20001048002	1
Euro OTC	Ethacridine lactate monoh…	2905007-01	1
Euro OTC	Ethacridine lactate monoh…	2905007v-03	1
Euro OTC	Ethacridine lactate monoh…	2905007V-03	1
Euro OTC	Ethacridine lactate monoh…	A201801002	1
Fagron	Ethacridine lactate monoh…	11/07-N05	1
Fagron	Ethacridine lactate monoh…	12/24-N04	2
Fagron	Ethacridine lactate monoh…	12324N03	1
Fagron	Ethacridine lactate monoh…	12A02-N10	1
Fagron	Ethacridine lactate monoh…	12C30-N07	1
Fagron	Ethacridine lactate monoh…	12G02-N13	5
Fagron	Ethacridine lactate monoh…	12G02-N135-15	1
Fagron	Ethacridine lactate monoh…	12J24-N04	1
Fagron	Ethacridine lactate monoh…	13/24-N03	5
Fagron	Ethacridine lactate monoh…	13/24-NO3	1
Fagron	Ethacridine lactate monoh…	13I24-N03	7
Fagron	Ethacridine lactate monoh…	13l24-N03	1
Fagron	Ethacridine lactate monoh…	1412034-04	1
Fagron	Ethacridine lactate monoh…	14A15-B04	2
Fagron	Ethacridine lactate monoh…	14A15-B04-300493	6
Fagron	Ethacridine lactate monoh…	16273411	1
Fagron	Ethacridine lactate monoh…	16e20-b11-322514	1
Fagron	Ethacridine lactate monoh…	16E20-B11-322514	5
Fagron	Ethacridine lactate monoh…	16E20-B11-326633	1
Fagron	Ethacridine lactate monoh…	16E20-B11-328430	1
Fagron	Ethacridine lactate monoh…	201205001	2
Finze	Ethacridine lactate monoh…	90601	1
Gehe amax	Ethacridine lactate monoh…	18314607	1
Gehe	Ethacridine lactate monoh…	13I24-N03	1
Gehe	Ethacridine lactate monoh…	141101	1
Gehe	Ethacridine lactate monoh…	1412034-03	1
Gehe	Ethacridine lactate monoh…	17247605	2
Gehe	Ethacridine lactate monoh…	21001424014	1
Gehe	Ethacridine lactate monoh…	22001737008	1
Kehr	Ethacridine lactate monoh…	22001737014	1
Kehr	Ethacridine lactate monoh…	22001737016	1
Liaoyuang Silver Eag…	Ethacridine lactate monoh…	1412034-02	1
Noweda	Ethacridine lactate monoh…	183146005	1
Noweda	Ethacridine lactate monoh…	18314601	1
Noweda	Ethacridine lactate monoh…	18314607	2
Noweda	Ethacridine lactate monoh…	20001048002	2
Noweda	Ethacridine lactate monoh…	22001737011	3
Noweda	Ethacridine lactate monoh…	3785846	1
phoenix 18.11.2014	Ethacridine lactate monoh…	13/24-N03	1
Phoenix	Ethacridine lactate monoh…	100201	1
Phoenix	Ethacridine lactate monoh…	1412034-03	1
Phoenix	Ethacridine lactate monoh…	22001737016	1
Phönix	Ethacridine lactate monoh…	111201	1
Phonix	Ethacridine lactate monoh…	13I24-N03	1
Phönix	Ethacridine lactate monoh…	20001048002	1
Rezepturlager - Verl…	Ethacridine lactate monoh…	121/15	1
Rezepturlager - Verl…	Ethacridine lactate monoh…	220/17	1
Sanacorp HST	Ethacridine lactate monoh…	17247605	1
Sanacorp/EuRho	Ethacridine lactate monoh…	1412034-03	1

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 235 616 spectra from 1515 *Apo-Ident* customers from a total of 49 159 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ethacridine lactate monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ethacridine lactate monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	280	0	201 804
Type C	0	445	6	235 616

The substance/substance group *Ethacridine lactate monohydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.8571 %)
Type C	100.0000 % (> 99.9007 %)	98.6696 % (> 98.0044 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20750	21265	6.17	150.05
21265	21265	0.00	148.28
21636	21265	8.45	151.69
22500	21265	11.34	149.47
22733	21265	12.84	148.32
23247	21265	11.95	150.01
26357	26357	0.00	159.60

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ethinylestradiol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20950-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ethinylestradiol; Ethinylestradiolum

Special notes

When selecting the *Ethinylestradiol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ethinylestradiol	6	2	19

Second-stage model

For differentiation of the substance/substance group *Ethinylestradiol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ethinylestradiol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	108.98	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ethinylestradiol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ethinylestradiol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ethinylestradiol	13I09-N04	20950	40	1402058
Fagron	Ethinylestradiol	14E15-B03-296049	21705	55	1507109
Fagron	Ethinylestradiol	14E15-B03-296049	21705SI	56	1507109
Fagron	Ethinylestradiol	14E15-B03-310270	21916	60	20140708
Fagron	Ethinylestradiol	14E15-B03-310270	21916SI	60	20140708
Fagron	Ethinylestradiol	14E15-B03-310270	21958	60	20140708
Fagron	Ethinylestradiol	18E25-B01-355721	24584	40	20180810
Fagron	Ethinylestradiol	19J11-F01-367137	25045	40	2007191
Fagron	Ethinylestradiol	22A18-F02-382202	26327	40	20220429
Fagron	Ethinylestradiol	22A18-F02-382202	26327SI	40	20220429

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 491 spectra of 10 reference samples from the substance/substance group *Ethinylestradiol*. These samples are listed above in the *calibration samples* section. The reference samples come from 6

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

different batches.

- 152 471 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 312 spectra of 7 reference samples from the substance/substance group *Ethinylestradiol*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ethinylestradiol	16B17-B01-329904	23075	40
Fagron	Ethinylestradiol	23E16-B04-234620	27053	40
Fagron	Ethinylestradiol	14E15-B03-310270	21958SI†	43
Fagron	Ethinylestradiol	16B17-B01-329904	23075SI	30
Fagron	Ethinylestradiol	18E25-B01-355721	24584SI†	40
Fagron	Ethinylestradiol	19J11-F01-367137	25045SI†	40
Fagron	Ethinylestradiol	23E16-B04-234620	27053SI	79

- 201 772 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 36 spectra from 28 *Apo-Ident* customers from 23 batches from the substance/substance group *Ethinylestradiol*.

- Among them are spectra of independent samples from 19 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
Caelo	Ethinylestradiol	18E25-B01-0001	1
Fagron	Ethinylestradiol	12D19-N04	1
Fagron	Ethinylestradiol	1367138	2
Fagron	Ethinylestradiol	13G03-N04	1
Fagron	Ethinylestradiol	13I09-N04	1
Fagron	Ethinylestradiol	14e15b03296049	1
Fagron	Ethinylestradiol	16B17-B01	1
Fagron	Ethinylestradiol	16B17-B01-320666	1
Fagron	Ethinylestradiol	16B17-B01-333326	1
Fagron	Ethinylestradiol	18E25-B01	2
Fagron	Ethinylestradiol	18E25-B01-351832	2
Fagron	Ethinylestradiol	18E25-B01-352721	1
Fagron	Ethinylestradiol	18E25-B01-353920	3
Fagron	Ethinylestradiol	18E25-B01-355721	4
Fagron	Ethinylestradiol	19J11-F01-367137	1
Fagron	Ethinylestradiol	19J11-F01-367138	5
Fagron	Ethinylestradiol	19J11-F01-373282	2
Fagron	Ethinylestradiol	22A18-F02-382202	1
Fagron	Ethinylestradiol	22A18-FO2-382202	1
Fagron	Ethinylestradiol	84100720	1
Fagron	Ethinylestradiol	8561175	1
Fagron	Ethinylestradiol	F01-3671308	1
Fagron	Ethinylestradiol	UN803HA	1

- 236 031 spectra from 1515 *Apo-Ident* customers from a total of 49 235 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ethinylestradiol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ethinylestradiol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	491	0	152 471
Type B	0	312	0	201 772
Type C	0	36	0	236 031

The substance/substance group *Ethinylestradiol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7780 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.0769 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 83.3333 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20950	20950	0.00	172.20
21705	21705	0.00	207.26
21916	21705	9.70	189.12
21958	21705	8.61	192.25
24584	20950	40.25	159.16
25045	25045	0.00	215.29
26327	20950	30.28	169.73

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ethosuximide**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	24100-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ethosuximide; Ethosuximidum

Special notes

When selecting the *Ethosuximide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ethosuximide	2	1	0

Second-stage model

For differentiation of the substance/substance group *Ethosuximide* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ethosuximide* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Menthol	73.65	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ethosuximide* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ethosuximide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Katwijk Ch...	Ethosuximide	451717	24100	40	20180509
Katwijk Ch...	Ethosuximide	451645	24101	40	1807457

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Ethosuximide*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

- 152 882 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Ethosuximide*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Katwijk Chemie BV	Ethosuximide	451644	24102	40

- 202 044 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Ethosuximide*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ethosuximide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ethosuximide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	80	0	152 882
Type B	0	40	0	202 044
Type C	0	0	0	236 067

The substance/substance group *Ethosuximide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24100	24101	31.68	118.58
24101	24101	0.00	120.43

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Fampridine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20902-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fampridine; Fampridinum

Special notes

When selecting the *Fampridine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Fampridine	9	5	46

Second-stage model

For differentiation of the substance/substance group *Fampridine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fampridine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	153.67	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Fampridine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Fampridine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fampridine	16276001	22881	40	20161024
Caelo	Fampridine	16276001	22905	40	20161024
Caelo	Fampridine	16276001	23074	40	20161024
Caelo	Fampridine	16276001	23237	40	20161024
Caelo	Fampridine	190675	24724	40	20190506*
Caelo	Fampridine	180219	24756	40	20180214*
Caelo	Fampridine	180219	24756SI	40	20180214*
Caelo	Fampridine	20003524	25559	40	20201126*
Caelo	Fampridine	20003524	25559SI	40	20201126*
Fagron	Fampridine	13G26-N06	20902	40	1402686
Fagron	Fampridine	14D11-B06-293750	21541	60	20140113
Fagron	Fampridine	16D11-B07-318220	22491	40	AR-16-FG-011566-01
Fagron	Fampridine	16E25-B03-324097	22894	40	20160609
Fagron	Fampridine	16E25-B03-324097	22945	40	20160609
Fagron	Fampridine	17K20-B02-349165	24439	40	20180103
Fagron	Fampridine	17K20-B02-349165	24439SI	40	20180103

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 660 spectra of 16 reference samples from the substance/substance group *Fampridine*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 302 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 435 spectra of 11 reference samples from the substance/substance group *Fampridine*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Fampridine	172170	23653	40
Caelo	Fampridine	19000755	25197	40
Caelo	Fampridine	22001045	26119	40
Fagron	Fampridine	19G24-B02-363769	24823	40
Fagron	Fampridine	22I21-B07-223809	26385	40
Caelo	Fampridine	190675	24724SI†	40
Caelo	Fampridine	19000755	25197SI	40
Caelo	Fampridine	22001045	26119SI	40
Fagron	Fampridine	16E25-B03-324097	22894SI†	40
Fagron	Fampridine	19G24-B02-363769	24823SI	35
Fagron	Fampridine	22I21-B07-223809	26385SI	40

- 201 649 spectra from a total of 4038 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 79 spectra from 24 *Apo-Ident* customers from 48 batches from the substance/substance group *Fampridine*.
- Among them are spectra of independent samples from 46 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Fampridine	22K17-B03-228705	1
	Fampridine	353033	1
Caelo	Fampridine	15350001	1
Caelo	Fampridine	15350002	1
Caelo	Fampridine	16276001	1
Caelo	Fampridine	16276002	3
Caelo	Fampridine	17217002	1
Caelo	Fampridine	17217003	2
Caelo	Fampridine	17217004	1
Caelo	Fampridine	17217005	1
Caelo	Fampridine	18021901	1
Caelo	Fampridine	18021903	2
Caelo	Fampridine	18021907	3
Caelo	Fampridine	19000755005	2
Caelo	Fampridine	19000755007	1
Caelo	Fampridine	19067501	1
Caelo	Fampridine	19067504	1
Caelo	Fampridine	24111801	1
Caesar & Loretz GmbH/Gehe	Fampridine	22001045001	2
Fagron	Fampridine	13C07-B02-289395	1
Fagron	Fampridine	14D11-B06-296110	1
Fagron	Fampridine	14D11-B40-301641	1
Fagron	Fampridine	14D11-B40-304961	1
Fagron	Fampridine	16/19-Bo4-330727	1
Fagron	Fampridine	16D11-B07	1
Fagron	Fampridine	17/19-B01	2
Fagron	Fampridine	17/19-B01-339467	1
Fagron	Fampridine	17D19-B01-333745	1
Fagron	Fampridine	17K20_B02_344609	1
Fagron	Fampridine	17K20-B02	4
Fagron	Fampridine	17K20-B02-344609	2
Fagron	Fampridine	17K20-B02-349165	1
Fagron	Fampridine	17K20-B02-349165/0000254876	1
Fagron	Fampridine	18121801	1
Fagron	Fampridine	18H01-B08	1
Fagron	Fampridine	19G24-B02	4
Fagron	Fampridine	19G24-B02-363768	5
Fagron	Fampridine	19g24-b02-363769	1
Fagron	Fampridine	19G24-B02-363770	9
Fagron	Fampridine	20D06-F07-370084	2
Fagron	Fampridine	20D06-F07-370086	2
Fagron	Fampridine	22C25-B07-215458	1
Fagron	Fampridine	22C25-B07-215459	1
Fagron	Fampridine	22k17-b03-226121	1
Fagron	Fampridine	254876	1
Inresa	Fampridine	220825	1
Inresa	Fampridine	236761	1
Noweda	Fampridine	17K20-B02-349165	1
PHÖNIX	Fampridine	20210217-2	1

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 235 988 spectra from 1515 *Apo-Ident* customers from a total of 49 210 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fampridine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fampridine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	660	0	152 302
Type B	0	435	0	201 649
Type C	0	78	1	235 988

The substance/substance group *Fampridine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0909 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6207 %)
Type C	100.0000 % (> 99.9007 %)	98.7342 % (> 94.9367 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20902	20902	0.00	268.63
21541	20902	7.36	271.04
22491	22491	0.00	293.16
22881	20902	33.50	271.48
22894	22491	7.58	290.23
22905	20902	31.26	272.02
22945	22491	12.03	288.27
23074	20902	35.25	271.18
23237	22491	36.60	271.82
24439	22491	7.95	293.36

continued on the next page

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24724	24724	0.00	266.49
24756	24756	0.00	267.37
25559	25559	0.00	255.62

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ferrous gluconate hydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	24166-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ferrous gluconate hydrate; Ferrosi gluconas hydricus

Special notes

When selecting the *Ferrous gluconate hydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ferrous gluconate hydrate	4	1	0

Second-stage model

For differentiation of the substance/substance group *Ferrous gluconate hydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ferrous gluconate hydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	108.35	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ferrous gluconate hydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ferrous gluconate hydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Ferrous gluconate hydrate	2008035	25378	40	20201015*
Euro OTC	Ferrous gluconate hydrate	2103004	25604	40	20210329*
Euro OTC	Ferrous gluconate hydrate	2201008	26085	40	20220425*
Euro OTC	Ferrous gluconate hydrate	2307024	26859	40	20230821*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 160 spectra of 4 reference samples from the substance/substance group *Ferrous gluconate hydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 802 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 3 reference samples from the substance/substance group *Ferrous gluconate hydrate*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ferrous gluconate hydrate	1805025	24166	40
Euro OTC	Ferrous gluconate hydrate	2201008	26085SI†	20
Euro OTC	Ferrous gluconate hydrate	2307024	26859SI†	20

- 202 004 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Ferrous gluconate hydrate*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Validation results

The validation runs checked whether the substance/substance group *Ferrous gluconate hydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ferrous gluconate hydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	160	0	152 802
Type B	0	80	0	202 004
Type C	0	0	0	236 067

The substance/substance group *Ferrous gluconate hydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25378	25378	0.00	410.06
25604	25604	0.00	400.53
26085	26085	0.00	401.96
26859	26859	0.00	400.04

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Finasteride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20955-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Finasteride; Finasteridum

Special notes

When selecting the *Finasteride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Finasteride	7	13	33

Second-stage model

For differentiation of the substance/substance group *Finasteride* the following second-stage model is used:

- Submodel 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Finasteride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	106.92	135.77
⋮	⋮	⋮
Riboflavin sodium phosphate hydrate	>50	163.56
Mg-Ca-K colamine phosphate	>50	360.86
Magnesium citrate	>50	361.34
Gentamicin sulfate	>50	786.20
Tobramycin sulfate	>50	969.08
Neomycin sulfate	>50	1163.29
Zinc gluconate	>50	1660.09
Sodium tetraborate	>50	2082.92

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Finasteride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Finasteride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Finasteride	1403016-01	21626	60	1506004
Euro OTC	Finasteride	1403016-02	21750	60	20140505
Euro OTC	Finasteride	1403016-02	21750SI	51	20140505
Euro OTC	Finasteride	1605020	22565	40	20160613*
Euro OTC	Finasteride	1605020	22565SI	40	20160613*
Euro OTC	Finasteride	1610012	22856	40	20161116*
Euro OTC	Finasteride	1610012	22856SI	33	20161116*
Euro OTC	Finasteride	2101024	25527	40	20210217*
Euro OTC	Finasteride	2101024	25527SI	34	20210217*
Fagron	Finasteride	13I03-N01	20955	40	1411272
Fagron	Finasteride	14A16-B40-295980	21742	60	20140317
Fagron	Finasteride	14A16-B40-295980	21742SI	45	20140317

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 543 spectra of 12 reference samples from the substance/substance group *Finasteride*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.
- 152 419 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1052 spectra of 27 reference samples from the substance/substance group *Finasteride*.
- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Finasteride	1704004	23151	40
Euro OTC	Finasteride	1804010	24129	40
Euro OTC	Finasteride	1809019	24342	40
Euro OTC	Finasteride	2003027	25355	40
Euro OTC	Finasteride	2111004	25913	40
Euro OTC	Finasteride	2210013	26421	40
Euro OTC	Finasteride	2210015	26438	40
Euro OTC	Finasteride	2301045	26576	40
Euro OTC	Finasteride	2403004	27291	40
Euro OTC	Finasteride	2407022	27367	30
Fagron	Finasteride	15J15-B02-320084	22594	40
Fagron	Finasteride	22B14-B09-217630	26078	40
Fagron	Finasteride	23J19-B04-233067	27039	40
Euro OTC	Finasteride	1804010	24129SI	40
Euro OTC	Finasteride	1809019	24342SI	31
Euro OTC	Finasteride	2003027	25355SI	39
Euro OTC	Finasteride	2111004	25913SI	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Finasteride	2210013	26421SI	40
Euro OTC	Finasteride	2210015	26438SI	40
Euro OTC	Finasteride	2301045	26576SI	40
Euro OTC	Finasteride	2403004	27291SI	40
Euro OTC	Finasteride	2407022	27367SI	38
Fagron	Finasteride	15J15-B02-320084	22594SI	40
Fagron	Finasteride	15J15-B02-320084	22595	40
Fagron	Finasteride	15J15-B02-320084	22595SI	40
Fagron	Finasteride	22B14-B09-217630	26078SI	40
Fagron	Finasteride	23J19-B04-233067	27039SI	34

- 201 032 spectra from a total of 4032 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 53 spectra from 19 *Apo-Ident* customers from 35 batches from the substance/substance group *Finasteride*.

- Among them are spectra of independent samples from 33 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Finasteride	17I12-B07-340606	1
Caelo	Finasteride	1809019-01	1
Crystal	Finasteride	141100801	1
Euro OTC	Finasteride	1403016-02	1
Euro OTC	Finasteride	1411008-01	1
Euro OTC	Finasteride	1605020-01	1
Euro OTC	Finasteride	1610012-01	2
Euro OTC	Finasteride	1704004-01	5
Euro OTC	Finasteride	1804010-01	2
Euro OTC	Finasteride	1809019-01	2
Euro OTC	Finasteride	18090919-01	1
Euro OTC	Finasteride	20B11-F03-373005	1
Euro OTC	Finasteride	2101024-01	1
Euro OTC	Finasteride	2210013-01	1
Euro OTC	Finasteride	C1012/116010	1
Fagron	Finasteride	13I03-N01	2
Fagron	Finasteride	14111305	1
Fagron	Finasteride	14L23-B02-306981	1
Fagron	Finasteride	15I01-B03	1
Fagron	Finasteride	15I01-B03-314476	1
Fagron	Finasteride	17011303	1
Fagron	Finasteride	17I12-B07-340606	4
Fagron	Finasteride	17I12-B07-355068	1
Fagron	Finasteride	17I12-B07-356321	1
Fagron	Finasteride	18041810	1
Fagron	Finasteride	18L13-B05-356320	1
Fagron	Finasteride	18L13-B05-356321	2
Fagron	Finasteride	19041707	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Finasteride	19D10-B01-362337	3
Fagron	Finasteride	20181101	1
Fagron	Finasteride	20190301	1
Fagron	Finasteride	20190702	1
Fagron	Finasteride	20B11-F03-373005	1
Fagron	Finasteride	20J01-F05-374980	1
Fagron	Finasteride	22B14-B09-217630	2
Fagron	Finasteride	F03-3730005	1
Phoenix	Finasteride	1804010-01	1
Shandong Northwest M...	Finasteride	FNA160604	1

- 236 014 spectra from 1515 *Apo-Ident* customers from a total of 49 223 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Finasteride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Finasteride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	543	0	152 419
Type B	0	1052	0	201 032
Type C	0	53	0	236 014

The substance/substance group *Finasteride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8950 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4297 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 88.6792 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20955	20955	0.00	187.42
21626	21626	0.00	179.27
21742	21626	24.73	178.64
21750	21626	20.63	177.74
22565	22565	0.00	182.69
22856	22856	0.00	185.55
25527	25527	0.00	188.58

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Fluocinolone acetonide**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21031-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fluocinolone acetonide; Fluocinoloni acetonidum

Special notes

When selecting the *Fluocinolone acetonide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Fluocinolone acetonide	6	3	43

Second-stage model

For differentiation of the substance/substance group *Fluocinolone acetonide* the following second-stage model is used:

- Submodel 02

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fluocinolone acetonide* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Triamcinolone acetonide	59.79	36.51
⋮	⋮	⋮
Betamethasone	>50	65.70
Dexamethasone	>50	73.91
Methylprednisolone	>50	82.43
Tyrothricin	>50	87.41
Prednisolone	>50	87.53
Gramicidin	>50	153.42

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Fluocinolone acetonide* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Fluocinolone acetonide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fluocinolone acetonide	12035003	21756	60	20120321
Caelo	Fluocinolone acetonide	12035003	21756SI	48	20120321
Caelo	Fluocinolone acetonide	162281	22637	40	20160907*
Caelo	Fluocinolone acetonide	162281	22637SI	30	20160907*
Euro OTC	Fluocinolone acetonide	2804013E-01	21031	60	1404008
Euro OTC	Fluocinolone acetonide	2804013E-01	21077	60	20121206
Euro OTC	Fluocinolone acetonide	2804013E-01	21822	60	20121206
Euro OTC	Fluocinolone acetonide	2804013E-01	21822SI	60	20121206
Fagron	Fluocinolone acetonide	14L19-B04-307101	22267	45	20150219
Fagron	Fluocinolone acetonide	14L19-B04-307101	22267SI	45	20150219
Fagron	Fluocinolone acetonide	14L19-B04-307101	23080	40	20150219
Fagron	Fluocinolone acetonide	17F14-B08-350105	24700	40	20171221
Fagron	Fluocinolone acetonide	20K03-F03-375403	25750	40	2111539
Fagron	Fluocinolone acetonide	20K03-F03-375403	25750SI	40	2111539

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 668 spectra of 14 reference samples from the substance/substance group *Fluocinolone acetonide*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 294 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 378 spectra of 10 reference samples from the substance/substance group *Fluocinolone acetonide*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Fluocinolone acetonide	172130	23674	40
Fagron	Fluocinolone acetonide	21K03-B06-217656	26069	40
Fagron	Fluocinolone acetonide	22D11-B02-221847	26325	40
Caelo	Fluocinolone acetonide	172130	23674SI	12
Euro OTC	Fluocinolone acetonide	2804013E-01	21823	60
Euro OTC	Fluocinolone acetonide	2804013E-01	21823SI	46
Fagron	Fluocinolone acetonide	14L19-B04-307101	23080SI†	20
Fagron	Fluocinolone acetonide	17F14-B08-350105	24700SI†	40
Fagron	Fluocinolone acetonide	21K03-B06-217656	26069SI	40
Fagron	Fluocinolone acetonide	22D11-B02-221847	26325SI	40

- 201 706 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 66 spectra from 42 *Apo-Ident* customers from 48 batches from the substance/substance group *Fluocinolone acetonide*.
- Among them are spectra of independent samples from 43 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Fluocinolone acetonide	22D11-B02-221848	1
	Fluocinolone acetonide	22D11-B02-221848	1
Caelo	Fluocinolone acetonide	12035003	1
Caelo	Fluocinolone acetonide	16228108	2
Caelo	Fluocinolone acetonide	18073203	1
Caelo	Fluocinolone acetonide	18073206	1
Caelo	Fluocinolone acetonide	18073303	2
Caelo	Fluocinolone acetonide	2804013V-03	1
Caesar & Loretz Hilden	Fluocinolone acetonide	18073301	1
Eurho	Fluocinolone acetonide	1408022-04	1
Euro OTC	Fluocinolone acetonide	1408022-02	4
Euro OTC	Fluocinolone acetonide	1408022-03	1
Euro OTC	Fluocinolone acetonide	2804013E-01	1
Fagro/Noweda	Fluocinolone acetonide	15K06-B02-336730	1
Fagron	Fluocinolone acetonide	1(18I19-B05-363303)	1
Fagron	Fluocinolone acetonide	13E22-N10	1
Fagron	Fluocinolone acetonide	13L30B35295489	1
Fagron	Fluocinolone acetonide	13L30-B35-295489	1
Fagron	Fluocinolone acetonide	14l19-b04	1
Fagron	Fluocinolone acetonide	14L19-B04	4
Fagron	Fluocinolone acetonide	14L19-B04-317248	2
Fagron	Fluocinolone acetonide	14L19-B04-615699	1
Fagron	Fluocinolone acetonide	15K06-B02	1
Fagron	Fluocinolone acetonide	15k06-b02-326488	1
Fagron	Fluocinolone acetonide	15k06-b02-332955	1
Fagron	Fluocinolone acetonide	15K06-B02-336730	1
Fagron	Fluocinolone acetonide	17f14-b08-346965	1
Fagron	Fluocinolone acetonide	17F14-B08-346965	1
Fagron	Fluocinolone acetonide	17F14-B08-350106	3
Fagron	Fluocinolone acetonide	18/19-B05-359031	1
Fagron	Fluocinolone acetonide	18/19-B05-365691	1
Fagron	Fluocinolone acetonide	18/19-B05-370559	1
Fagron	Fluocinolone acetonide	18I19B05-358085	1
Fagron	Fluocinolone acetonide	18I19-B05-358085	2
Fagron	Fluocinolone acetonide	18I19-B05-363303	1
Fagron	Fluocinolone acetonide	18I19-B05-365691	1
Fagron	Fluocinolone acetonide	2151nm1b0091723	1
Fagron	Fluocinolone acetonide	2151NM1B0091723	2
Fagron	Fluocinolone acetonide	21H13-B18-213858	2
Fagron	Fluocinolone acetonide	21K03-B06	2
Fagron	Fluocinolone acetonide	22D11-B02-221848	1
Fagron	Fluocinolone acetonide	B05-3590301	1
Fagron	Fluocinolone acetonide	B05-3633003	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Fluocinolone acetonide	B05-3705509	1
Fargon/Kehr	Fluocinolone acetonide	14L-19-B04	1
Fargon/Noweda	Fluocinolone acetonide	13L13-B35	1
Farmabios s.p.A	Fluocinolone acetonide	C24H30F206	1
Gehe	Fluocinolone acetonide	18/19-B05	1
Ichthyol Gesellschaf…	Fluocinolone acetonide	14L19-B04-321003	1
Kehr	Fluocinolone acetonide	17F14-B08-346965	1
Noweda	Fluocinolone acetonide	23D01-B03-231001	1

- 236 001 spectra from 1515 *Apo-Ident* customers from a total of 49 210 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fluocinolone acetonide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fluocinolone acetonide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	668	0	152 294
Type B	0	378	0	201 706
Type C	0	66	0	236 001

The substance/substance group *Fluocinolone acetonide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1018 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.4127 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 90.9091 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21031	21031	0.00	63.04
21077	21031	4.38	63.96
21756	21031	22.59	62.97
21822	21031	19.63	64.63
22267	21031	17.79	62.87
22637	22637	0.00	119.13
23080	21031	20.38	59.79
24700	21031	11.30	60.27
25750	25750	0.00	113.86

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Folic acid hydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20370-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Folic acid hydrate; Acidum folicum hydricum

Special notes

When selecting the *Folic acid hydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Folic acid hydrate	7	6	16

Second-stage model

For differentiation of the substance/substance group *Folic acid hydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Folic acid hydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	93.44	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Folic acid hydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Folic acid hydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Folic acid hydrate	1401005-01	21288	40	20140131
Euro OTC	Folic acid hydrate	1508024	21891	60	20150902*
Euro OTC	Folic acid hydrate	1604036	22554	40	20160429*
Euro OTC	Folic acid hydrate	1611009	22868	40	20161201*
Euro OTC	Folic acid hydrate	1911019	25072	40	20191216*
Fagron	Folic acid hydrate	12G17-N05	20767	40	20120727
Fagron	Folic acid hydrate	16C03-B06-322513	23081	40	20160411

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 300 spectra of 7 reference samples from the substance/substance group *Folic acid hydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 662 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 290 spectra of 9 reference samples from the substance/substance group *Folic acid hydrate*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Folic acid hydrate	1608030	22818	40
Euro OTC	Folic acid hydrate	1903033	24608	40
Euro OTC	Folic acid hydrate	2006021	25272	40
Euro OTC	Folic acid hydrate	2201042	25964	40
Euro OTC	Folic acid hydrate	2312005	27196	40
Euro OTC	Folic acid hydrate	2407015	27361	40
Euro OTC	Folic acid hydrate	2201042	25964SI	10
Euro OTC	Folic acid hydrate	2312005	27196SI	20
Euro OTC	Folic acid hydrate	2407015	27361SI	20

- 201 794 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 27 spectra from 20 *Apo-Ident* customers from 17 batches from the substance/substance group *Folic acid hydrate*.

- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
EuRho	Folic acid hydrate	1911019-01	1
Euro OTC	Folic acid hydrate	1307041-01	1
Euro OTC	Folic acid hydrate	1401005-01	1
Euro OTC	Folic acid hydrate	1604036-01	1
Euro OTC	Folic acid hydrate	1608030-01	1
Euro OTC	Folic acid hydrate	1611009-01	5
Euro OTC	Folic acid hydrate	1611009-02	1
Euro OTC	Folic acid hydrate	1611009-04	1
Euro OTC	Folic acid hydrate	1903033-01	2
Euro OTC	Folic acid hydrate	1911019-01	2
Euro OTC	Folic acid hydrate	2006021-01	1
Euro OTC	Folic acid hydrate	2201042-01	1
Fagron	Folic acid hydrate	13A11-N01	1
Fagron	Folic acid hydrate	13G16-N02	4
Fagron	Folic acid hydrate	14H05-B03	1
Fagron	Folic acid hydrate	16C03-B06	1
Fagron	Folic acid hydrate	UT11110182	1
Farmalabor	Folic acid hydrate	P1701610	1

- 236 040 spectra from 1515 *Apo-Ident* customers from a total of 49 241 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Folic acid hydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Folic acid hydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	290	0	201 794
Type C	0	27	0	236 040

The substance/substance group *Folic acid hydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.9310 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 77.7778 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20767	22554	4.69	116.74
21288	22554	4.54	115.98
21891	21891	0.00	113.77
22554	22554	0.00	113.72
22868	22868	0.00	113.22
23081	22554	4.51	111.08
25072	25072	0.00	115.97

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Fructose**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20074-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fructose; Fructosum

Special notes

When selecting the *Fructose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Fructose	7	21	289

Second-stage model

For differentiation of the substance/substance group *Fructose* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fructose* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	62.28	41.66
⋮	⋮	⋮
Calcium glycerophosphate	>50	35.61
Riboflavin	>50	40.22
Colistin sulfate	>50	41.45
Amphotericin B	>50	49.72
Tosylchloramide sodium	>50	56.26
Bacitracin	>50	57.74
SyrSpend® SF pH4 neo (Maize starch)	>50	61.09
Wheat starch	>50	64.33
Rice starch	>50	64.96
Calcium pantothenate	>50	65.30
SyrSpend® SF Alka	>50	68.05
Potato starch	>50	74.95
Nystatin	>50	77.90
Selenium yeast	>50	78.65
SyrSpend® SF pH4	>50	79.21
Gelatine, white	>50	84.34
Carmellose sodium	>50	85.76
Maltodextrin	>50	88.82
Acacia, dried dispersion	>50	91.47
Corn starch	>50	99.85
Triamcinolone	>50	99.92
Hyoscine hydrobromide	>50	103.24
Cyanocobalamin	>50	108.64
Oxalic acid	>50	110.73
Estradiol hemihydrate	>50	112.00
Methylcobalamin	>50	161.71
alpha-tocopheryl acetate dry concentrate	>50	168.94
Estriol	>50	169.06

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Fructose* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Fructose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Fructose	160667	22481	60	20160425*
Caelo	Fructose	15084311	22490	40	20150316
Euro OTC	Fructose	1212015-01	21281	40	20130111
Euro OTC	Fructose	1509037	21934	60	20151027*
Euro OTC	Fructose	1512009	22292	60	20160113*
Euro OTC	Fructose	1701049	22986	40	20170213*
Fagron	Fructose	16H05-B01-326259	23018	40	20160926
Fagron	Fructose	16H05-B01-326259	23082	40	20160926

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 380 spectra of 8 reference samples from the substance/substance group *Fructose*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.
- 152 582 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 921 spectra of 25 reference samples from the substance/substance group *Fructose*.
- Among them are spectra of independent samples from 21 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Fructose	15271213	22583	40
Caelo	Fructose	171439	23422	40
Caelo	Fructose	182916	24364	40
Caelo	Fructose	191699	24739	40
Caelo	Fructose	21000686007	25931	40
Caelo	Fructose	23002084	27334	40
Euro OTC	Fructose	1604024	22547	41
Euro OTC	Fructose	1607030	22693	40
Euro OTC	Fructose	1705002	23391	40
Euro OTC	Fructose	1710034	23901	40
Euro OTC	Fructose	1803040	24087	40
Euro OTC	Fructose	1811018	24486	40
Euro OTC	Fructose	1906017	24792	40
Euro OTC	Fructose	1910020	24978	40
Euro OTC	Fructose	2006019	25298	40
Euro OTC	Fructose	2102008	25602	40
Euro OTC	Fructose	2203030	26037	40
Euro OTC	Fructose	2212011	26516	40
Euro OTC	Fructose	2309017	26996	40
Euro OTC	Fructose	2405018	27281	40
Fagron	Fructose	19C19-B02-361846	25057	40
Caelo	Fructose	171439	23673	40
Caelo	Fructose	21000686007	25931SI	10
Euro OTC	Fructose	2203030	26037SI	10
Euro OTC	Fructose	2212011	26516SI	20

- 201 163 spectra from a total of 4024 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1268 spectra from 321 *Apo-Ident* customers from 293 batches from the substance/substance group *Fructose*.
- Among them are spectra of independent samples from 289 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Fructose	2006019-02	2
	Fructose	2100068018	1
	Fructose	21000686027	1
	Fructose	22003150003	10
	Fructose	22003150007	1
	Fructose	22003150009	1
	Fructose	22003150016	2
	Fructose	22003150021	3
	Fructose	2200315003	1
	Fructose	2203030-01	2
	Fructose	2203030-02	1
	Fructose	2212011-01	6
	Fructose	2212011-02	4
	Fructose	23003368001	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Fructose	23003368002	1
	Fructose	2309017-01	2
	Fructose	FS2P00251808-S02	1
AHD	Fructose	FS2P00252305-190	1
Alliance Health 13.0…	Fructose	13C25-N03	1
Alliance health	Fructose	14E01-B04-293505	2
Alliance health	Fructose	14K17-B99-300913	3
Alliance	Fructose	22003150002	2
Alliance	Fructose	2212011-01	1
Anzag	Fructose	18291602	1
apo-ident	Fructose	1607030-01	2
Beiersdorf	Fructose	14096208	1
Bombastus	Fructose	1710034-01	1
Caelo	Fructose	10051401	1
Caelo	Fructose	10071201	1
Caelo	Fructose	10087516	1
Caelo	Fructose	10381011	1
Caelo	Fructose	104H20	1
Caelo	Fructose	1081501	1
Caelo	Fructose	11071201	1
Caelo	Fructose	1114A03394	1
Caelo	Fructose	11258611	1
Caelo	Fructose	11258614	1
Caelo	Fructose	11258627	3
Caelo	Fructose	11258628	2
Caelo	Fructose	11I07-N06	1
Caelo	Fructose	12132301	2
Caelo	Fructose	12132305	5
Caelo	Fructose	12132309	2
Caelo	Fructose	12132310	1
Caelo	Fructose	12132313	5
Caelo	Fructose	12132314	5
Caelo	Fructose	12132317	2
Caelo	Fructose	12132320	1
Caelo	Fructose	12132322	2
Caelo	Fructose	12132325	3
Caelo	Fructose	121e29-n08	1
Caelo	Fructose	123456	1
Caelo	Fructose	1234567	1
Caelo	Fructose	12H01-N03	1
Caelo	Fructose	13041802	1
Caelo	Fructose	1309213394	1
Caelo	Fructose	13098902	3
Caelo	Fructose	13098904	1
Caelo	Fructose	13098906	4
Caelo	Fructose	13098909	1
Caelo	Fructose	13098911	1
Caelo	Fructose	13098913	4
Caelo	Fructose	13098914	2
Caelo	Fructose	13098915	1
Caelo	Fructose	13098917	3
Caelo	Fructose	13098918	1
Caelo	Fructose	13098922	1
Caelo	Fructose	130998922	1
Caelo	Fructose	13111705	1
Caelo	Fructose	13A28-N01	1
Caelo	Fructose	13E27-N07	1
Caelo	Fructose	14096201	2
Caelo	Fructose	14096202	1
Caelo	Fructose	14096203	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Fructose	14096205	3
Caelo	Fructose	14096207	1
Caelo	Fructose	14096208	2
Caelo	Fructose	14096210	1
Caelo	Fructose	14096211	1
Caelo	Fructose	14096219	4
Caelo	Fructose	14096223	5
Caelo	Fructose	14096224	2
Caelo	Fructose	14305201	1
Caelo	Fructose	14305203	2
Caelo	Fructose	14305204	1
Caelo	Fructose	14305206	1
Caelo	Fructose	14E01-B04-297098	1
Caelo	Fructose	1503045-01	2
Caelo	Fructose	15049703	1
Caelo	Fructose	15084301	3
Caelo	Fructose	15084305	3
Caelo	Fructose	15084308	2
Caelo	Fructose	15084311	2
Caelo	Fructose	15084312	2
Caelo	Fructose	1509037-01	2
Caelo	Fructose	152711201	1
Caelo	Fructose	15271201	3
Caelo	Fructose	15271205	7
Caelo	Fructose	15271208	2
Caelo	Fructose	15271209	4
Caelo	Fructose	15271213	6
Caelo	Fructose	15271214	2
Caelo	Fructose	15271215	3
Caelo	Fructose	15A16-B07	1
Caelo	Fructose	15A16-B07-305241	1
Caelo	Fructose	15A16-B07-308950	2
Caelo	Fructose	1604024-01	1
Caelo	Fructose	16066101	2
Caelo	Fructose	16066103	6
Caelo	Fructose	16066106	20
Caelo	Fructose	16066107	9
Caelo	Fructose	1607030-01	1
Caelo	Fructose	1610033-01	2
Caelo	Fructose	16283910	7
Caelo	Fructose	17007701	5
Caelo	Fructose	17007702	1
Caelo	Fructose	17007706	1
Caelo	Fructose	17007707	2
Caelo	Fructose	17007708	1
Caelo	Fructose	1701034-01	1
Caelo	Fructose	170104901	1
Caelo	Fructose	1705002-01	1
Caelo	Fructose	1710034-01	3
Caelo	Fructose	17143902	12
Caelo	Fructose	1714390210087516	1
Caelo	Fructose	17143903	2
Caelo	Fructose	17143904	10
Caelo	Fructose	17346404	29
Caelo	Fructose	17346405	1
Caelo	Fructose	17346405P-180831-1	1
Caelo	Fructose	17346405P-190325-2	1
Caelo	Fructose	17346405P-190718-1	1
Caelo	Fructose	17346406	1
Caelo	Fructose	17346411	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Fructose	18021501	1
Caelo	Fructose	1803040-01	4
Caelo	Fructose	18061801	1
Caelo	Fructose	18062005	1
Caelo	Fructose	18082002	9
Caelo	Fructose	18082005	38
Caelo	Fructose	18082006	1
Caelo	Fructose	18082011	4
Caelo	Fructose	18082012	4
Caelo	Fructose	1811018-01	1
Caelo	Fructose	1829102	1
Caelo	Fructose	18291602	40
Caelo	Fructose	18291603	1
Caelo	Fructose	18291603P-191223-2	1
Caelo	Fructose	18291605	2
Caelo	Fructose	18291609	7
Caelo	Fructose	18291611P-200319-9	1
Caelo	Fructose	18291612	2
Caelo	Fructose	18291613	5
Caelo	Fructose	18291614	1
Caelo	Fructose	18291620	2
Caelo	Fructose	1906017-01	7
Caelo	Fructose	1910020-01	2
Caelo	Fructose	191699005	1
Caelo	Fructose	19169903	13
Caelo	Fructose	19169904	8
Caelo	Fructose	19169905	1
Caelo	Fructose	192965002	7
Caelo	Fructose	192965008	16
Caelo	Fructose	192965009	1
Caelo	Fructose	20003599001	2
Caelo	Fructose	20003599011	5
Caelo	Fructose	20003599012	6
Caelo	Fructose	20081402	1
Caelo	Fructose	2100066022	1
Caelo	Fructose	21000686003	1
Caelo	Fructose	21000686007	5
Caelo	Fructose	21000686009	2
Caelo	Fructose	21000686015	5
Caelo	Fructose	21000686016	1
Caelo	Fructose	21000686018	2
Caelo	Fructose	21000686020	3
Caelo	Fructose	21000686022	11
Caelo	Fructose	21000686024	8
Caelo	Fructose	2102008-02	3
Caelo	Fructose	21051303	1
Caelo	Fructose	2117E-03394	1
Caelo	Fructose	22003150002	4
Caelo	Fructose	22003150003	3
Caelo	Fructose	22003150007	4
Caelo	Fructose	220425C	1
Caelo	Fructose	23021708	1
Caelo	Fructose	31031401	1
Caelo	Fructose	31101810	1
Caelo	Fructose	3313U-03394	1
Caelo	Fructose	5061503	1
Caelo	Fructose	5081701	1
Caelo	Fructose	7051304	1
Caelo	Fructose	7111401	1
Caelo	Fructose	716090F	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Fructose	9031504	1
Caelo	Fructose	9061804	1
Caelo	Fructose	92965008	1
Caesar & Loretz / Gehe	Fructose	18082012	1
Caesar & Loretz GmbH...	Fructose	19169904	1
Caesar & Loretz GmbH...	Fructose	18291605	2
Caesar & Loretz GmbH...	Fructose	18291613	2
Caesar & Loretz GmbH...	Fructose	20003599012	1
Caesar & Loretz GmbH...	Fructose	18291602	1
Caesar & Loretz GmbH...	Fructose	18291609	1
Caesar & Loretz GmbH/AHD	Fructose	18291602	1
Caesar & Loretz GmbH...	Fructose	21000686027	1
Caesar & Loretz GmbH/Gehe	Fructose	20003599011	1
Caesar & Loretz GmbH/Gehe	Fructose	21000686022	1
Caesar & Loretz GmbH...	Fructose	18082012	1
Caesar & Loretz GmbH...	Fructose	20003599001	1
Caesar & Loretz GmbH...	Fructose	18291602	1
Caesar & Loretz GmbH...	Fructose	19169904	4
Caesar & Loretz GmbH	Fructose	16283910	1
Caesar & Loretz GmbH	Fructose	18082005	4
Caesar & Loretz GmbH	Fructose	18082011	1
Caesar & Loretz GmbH	Fructose	18291602	24
Caesar & Loretz GmbH	Fructose	18291609	2
Caesar & Loretz GmbH	Fructose	18291613	1
Caesar & Loretz GmbH	Fructose	18307407	1
Caesar & Loretz GmbH	Fructose	191699008	1
Caesar & Loretz GmbH	Fructose	19169903	6
Caesar & Loretz GmbH	Fructose	19169904	1
Caesar & Loretz GmbH	Fructose	19169905	1
Caesar & Loretz GmbH	Fructose	192965002	8
Caesar & Loretz GmbH	Fructose	192965008	4
Caesar & Loretz GmbH	Fructose	20003599001	1
Caesar & Loretz GmbH	Fructose	20003599011	4
Caesar & Loretz GmbH	Fructose	20003599012	1
Caesar & Loretz GmbH	Fructose	21000686007	6
Caesar & Loretz GmbH	Fructose	21000686009	2
Caesar & Loretz GmbH	Fructose	21000686015	1
Caesar & Loretz GmbH	Fructose	21000686016	1
Caesar & Loretz GmbH	Fructose	21000686020	1
Caesar & Loretz GmbH	Fructose	21000686022	3
Caesar & Loretz GmbH	Fructose	21000686024	1
Caesar & Loretz GmbH	Fructose	22003150003	1
Caesar & Loretz GmbH	Fructose	22003150007	1
Caesar & Loretz/Geil...	Fructose	18291602	1
Caesar u. Loretz GmbH	Fructose	18082002	1
Caesar u. Loretz GmbH	Fructose	19169904	1
Caesar&Loretz/Noweda	Fructose	18082005	1
Ebert & Jacobi 08.08.16	Fructose	1604024-01	1
Eigen	Fructose	122F21	1
Eigen	Fructose	127D21	1
Eigen	Fructose	128I20	1
Eigenherstellung Defektur	Fructose	5082101	1
Eigenherstellung	Fructose	112K21	1
EuRho / Fiebig	Fructose	1910020-01	1
EuRho/Alliance	Fructose	2006019-01	2
Eurho/Gehe	Fructose	190601701	1
EuRho/Noweda	Fructose	1604024-01	1
EuRho	Fructose	1503045-01	1
EuRho	Fructose	1509037-01	4
EuRho	Fructose	1705002-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho	Fructose	171003401	2
EuRho	Fructose	1803040-01	1
EuRho	Fructose	2006019-19	1
Euro OTC	Fructose	1201017-01	2
Euro OTC	Fructose	1205022-01	1
Euro OTC	Fructose	1209010-01	1
Euro OTC	Fructose	121201-01pzn	1
Euro OTC	Fructose	1212015-01	2
Euro OTC	Fructose	12E29-N08	1
Euro OTC	Fructose	1307022-01	4
Euro OTC	Fructose	140100401	1
Euro OTC	Fructose	1401004-01	4
Euro OTC	Fructose	141000901	2
Euro OTC	Fructose	1410009-01	6
Euro OTC	Fructose	148890	1
Euro OTC	Fructose	1503045-01	7
Euro OTC	Fructose	1509037-01	7
Euro OTC	Fructose	1512009-01	9
Euro OTC	Fructose	1604024-01	4
Euro OTC	Fructose	1607030-01	17
Euro OTC	Fructose	1610033	1
Euro OTC	Fructose	1610033-01	12
Euro OTC	Fructose	1701049-01	14
Euro OTC	Fructose	170500201	1
Euro OTC	Fructose	1705002-01	10
Euro OTC	Fructose	171003401	1
Euro OTC	Fructose	1710034-01	33
Euro OTC	Fructose	180304001	1
Euro OTC	Fructose	1803040-01	34
Euro OTC	Fructose	1803040-012	1
Euro OTC	Fructose	1803040-02	3
Euro OTC	Fructose	1803040-03	1
Euro OTC	Fructose	1803040-1	1
Euro OTC	Fructose	18082002	1
Euro OTC	Fructose	181018-01	1
Euro OTC	Fructose	1811018	1
Euro OTC	Fructose	1811018-01	38
Euro OTC	Fructose	19006017-01	1
Euro OTC	Fructose	1906017-01	28
Euro OTC	Fructose	1910020-01	22
Euro OTC	Fructose	2006019-01	18
Euro OTC	Fructose	2102008-002	1
Euro OTC	Fructose	2102008-01	15
Euro OTC	Fructose	2102008-02	6
Euro OTC	Fructose	2203030_01	1
Euro OTC	Fructose	220303001	3
Euro OTC	Fructose	2203030-01	17
Euro OTC	Fructose	2212011-02	2
Euro OTC	Fructose	252207-4204	1
Euro OTC	Fructose	2731	1
Euro OTC	Fructose	AD15190330	1
Euro OTC	Fructose	AD16C91215	1
Euro OTC	Fructose	FS2P00251707-304	1
Euro OTC	Fructose	FS2P00251802-122	1
euro//Noweda	Fructose	1509037-01	1
euro//Noweda	Fructose	1710034-01	1
Euro/Gehe	Fructose	1604024-01	1
Euro/Gehe	Fructose	1607030-01	1
Euro/Krieger	Fructose	1906017-01	2
Euro/Noweda	Fructose	1610033-01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
euroct/gehe	Fructose	1212015-01	1
Europh/Ph	Fructose	1906017-01	1
Europh/Ph	Fructose	1910020-01	2
Fagron	Fructose	1107-N06	1
Fagron	Fructose	1170	1
Fagron	Fructose	12A26-N04	1
Fagron	Fructose	12E29-N08	3
Fagron	Fructose	12H01-N03	1
Fagron	Fructose	12Ho1-N03	1
Fagron	Fructose	12K28-N06	2
Fagron	Fructose	13098906	1
Fagron	Fructose	1312A-03394	1
Fagron	Fructose	13A28-N01	10
Fagron	Fructose	13C25-N03	3
Fagron	Fructose	13E27-n07	1
Fagron	Fructose	13E27-N07	2
Fagron	Fructose	13J18-B06	2
Fagron	Fructose	13J18-B06-286894	1
Fagron	Fructose	13J18B06286896	1
Fagron	Fructose	13J18-B06-286899	1
Fagron	Fructose	13J18-B06-292061	1
Fagron	Fructose	14E01-B04	3
Fagron	Fructose	14E01-B04-29350	1
Fagron	Fructose	14E01-B04-293505	6
Fagron	Fructose	14E01B04293506	1
Fagron	Fructose	14E01-B04-297098	2
Fagron	Fructose	14E1-B04-293506	1
Fagron	Fructose	14k17-B99	2
Fagron	Fructose	14K17-B99	2
Fagron	Fructose	14K17-B99-300913	1
Fagron	Fructose	15/21-B01	1
Fagron	Fructose	15/21-B01-312700	1
Fagron	Fructose	15/21-B01-323021	1
Fagron	Fructose	1521-B01-323021	1
Fagron	Fructose	15A16-B07	1
Fagron	Fructose	15A16-B07-303124	2
Fagron	Fructose	15A16-B07-305241	1
Fagron	Fructose	15A16-B07-308950	1
Fagron	Fructose	15I21-B01	1
Fagron	Fructose	15I21-B01-323020	1
Fagron	Fructose	15I21-B01-323021	5
Fagron	Fructose	15l21-B01-312701	2
Fagron	Fructose	15l21-B01-323021	1
Fagron	Fructose	16H05-B01	2
Fagron	Fructose	16H05-B01-326259	1
Fagron	Fructose	16H05-B01-330164	3
Fagron	Fructose	17007701	1
Fagron	Fructose	1705002-01	1
Fagron	Fructose	18082005	1
Fagron	Fructose	181018-01	1
Fagron	Fructose	1910020-01	1
Fagron	Fructose	19C19-B02-361846	1
Fagron	Fructose	3014Q-03394	1
Fagron	Fructose	326259	1
Fagron	Fructose	508Q-03394	1
Fagron	Fructose	516Q-03394	1
Fagron	Fructose	5217M-03394	1
Fagron	Fructose	7K21-N12	1
Fagron	Fructose	FR1413072	1
Fagron	Fructose	FR1443072	8

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Fructose	FR1713142	2
Fagron	Fructose	K43537721	2
Fargon	Fructose	14E01-B04-293506	2
Fargon	Fructose	15I21-B01-312701	1
Fiebig	Fructose	19169903	1
Finteler Apotheke	Fructose	16283910	1
fragon	Fructose	FR1413072	1
Gatt Koller	Fructose	1544/05141914	1
Gatt-Koller / Phoenix	Fructose	3156/0813	1
GEHE 17.06.2014	Fructose	13098913	1
Gehe	Fructose	1607030-01	2
Gehe	Fructose	17346404	1
GEHE	Fructose	1803040-01	2
Gehe	Fructose	18082005	1
Gehe	Fructose	1906017-01	1
Gehe	Fructose	2006019-01	1
gehe	Fructose	210200802	1
Gehe	Fructose	22003150021	2
gehe	Fructose	2203030-01	2
Gehe	Fructose	23003367001	1
Geilenkirchen	Fructose	17007707	1
Geilenkirchen	Fructose	17143904	1
Geilenkirchen	Fructose	18082012	1
Geilenkirchen	Fructose	180822	1
Geilenkirchen	Fructose	18291613	7
Geilenkirchen	Fructose	19169904	2
Jenne	Fructose	14A16-B07	1
Jenne	Fructose	15A16-B07	1
JENNE	Fructose	17L22-B02	2
Lihn/Reformhaus	Fructose	713E-03394	2
Nachprüfung	Fructose	1906017-01	1
Noweda	Fructose	1205022-01	1
Noweda	Fructose	16283910	1
Noweda	Fructose	1710034-01	4
Noweda	Fructose	17143902	1
Noweda	Fructose	1906017-01	2
Noweda	Fructose	1910020-01	2
Noweda	Fructose	19169903	1
Noweda	Fructose	20003599001	1
Noweda	Fructose	2003150015	1
Noweda	Fructose	2203030-02	1
Noweda	Fructose	FS2P00251808-502	1
Phoenix 05.08.2014	Fructose	FR1336122	3
Phoenix 11.12.2018	Fructose	1803040-01	1
Phoenix 17.11.19	Fructose	1803044-01	1
Phoenix 22.12.14	Fructose	1307022-01	1
Phoenix 22.12.14	Fructose	1401004-01	1
Phoenix	Fructose	15I21-B01	1
phoenix	Fructose	1906017-01	1
Phoenix	Fructose	1906017-01	1
Phoenix	Fructose	21000686015	1
Phönisx	Fructose	18291602	1
Phönix 17.05.2019	Fructose	1811018-01	2
Phönix Euro	Fructose	FS2P00251707-304	1
Phönix	Fructose	12K28-N06	1
PHÖNIX	Fructose	1710034-01	1
PHÖNIX	Fructose	17L22-B02-346104	1
Sanacorp	Fructose	17346404	1
SANACORP	Fructose	1811018-01	2
Sanacorp	Fructose	2212011-01	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Fructose	K43537721	1
Synopharm	Fructose	202A052	1

- 234 799 spectra from 1515 *Apo-Ident* customers from a total of 48 971 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fructose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fructose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	921	0	201 163
Type C	0	1267	1	234 799

The substance/substance group *Fructose* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.3485 %)
Type C	100.0000 % (> 99.9007 %)	99.9211 % (> 99.6845 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21281	22481	11.28	93.87
21934	21934	0.00	90.26
22292	22292	0.00	90.08
22481	22481	0.00	91.42

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22490	22292	5.26	91.22
22986	22986	0.00	89.52
23018	22292	5.74	90.82
23082	22481	7.11	91.25

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Furosemide**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20944-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Furosemide; Furosemidum

Special notes

When selecting the *Furosemide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Furosemide	6	3	29

Second-stage model

For differentiation of the substance/substance group *Furosemide* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Furosemide* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	157.47	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Furosemide* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Furosemide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Furosemide	13A22-N08	20944	40	1401379
Fagron	Furosemide	14K10-B02-301746	21819	60	20141215
Fagron	Furosemide	17D06-B01-338982	23940	40	20170626
Fagron	Furosemide	19I27-F04-366906	25044	40	20191218
Fagron	Furosemide	22L05-B06-225369	26607	40	20230104
Fagron	Furosemide	22L05-B06-225369	26607SI	20	20230104
Fagron	Furosemide	23G05-B14-230372	26977	40	20230830

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 7 reference samples from the substance/substance group *Furosemide*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 682 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 6 reference samples from the substance/substance group *Furosemide*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Furosemide	16B15-B06-322860	23083	40
Fagron	Furosemide	20G10-F10-373076	25442	40
Fagron	Furosemide	21K30-B02-221074	26168	40
Fagron	Furosemide	16B15-B06-322860	23084	40
Fagron	Furosemide	21K30-B02-221074	26168SI	20
Fagron	Furosemide	23G05-B14-230372	26977SI†	20

- 201 884 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 74 spectra from 56 *Apo-Ident* customers from 35 batches from the substance/substance group *Furosemide*.
- Among them are spectra of independent samples from 29 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Furosemide	20G10-F10-373076	1
	Furosemide	20G10-F10-374131	2
	Furosemide	-23201008	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
	Furosemide	23G05-B14230372	1
	Furosemide	23G05-B14-230372	1
AHC	Furosemide	23G05-B14-230372	1
Alliance Healthcare/…	Furosemide	12/13-N06	1
Caelo	Furosemide	16B15-B06	1
Caelo	Furosemide	20G10-F10-374131	1
Fagron	Furosemide	1095H2RI	1
Fagron	Furosemide	11K21-N26	1
Fagron	Furosemide	12A18-N03	1
Fagron	Furosemide	12I13-No6	1
Fagron	Furosemide	13A22-N08	4
Fagron	Furosemide	13E28-B40	2
Fagron	Furosemide	13E28-B40-289433	1
Fagron	Furosemide	13E28-B40-295538	1
Fagron	Furosemide	14K10-B02-301746	1
Fagron	Furosemide	15L10B02316506	1
Fagron	Furosemide	15L10-B02-316506	2
Fagron	Furosemide	16/26-B04-329253	2
Fagron	Furosemide	17d06-b01-335672	1
Fagron	Furosemide	17D06-B01-335672	2
Fagron	Furosemide	17D06-B01-338982	1
Fagron	Furosemide	18C27-B02	1
Fagron	Furosemide	18C27-B02-348148	2
Fagron	Furosemide	19I27-F04-366906	2
Fagron	Furosemide	-20200004	1
Fagron	Furosemide	20G10-F10	5
Fagron	Furosemide	20G10-F10-3730706	2
Fagron	Furosemide	20G10-F10373076	1
Fagron	Furosemide	20G10-F10-373076	16
Fagron	Furosemide	20G10-F10-373079	1
Fagron	Furosemide	20G10-F10-374131	3
Fagron	Furosemide	AM20216066	1
Fagron	Furosemide	F10-3730706	1
Fagron	Furosemide	FRD-2B-202004	2
Fagron	Furosemide	FUR-1A-192016	1
IPCA/Noweda	Furosemide	11D29-N08	1
Phoenix	Furosemide	17D06-B01-338982	1
Sanacorp	Furosemide	FUR-1A-192016	1

- 235 993 spectra from 1515 *Apo-Ident* customers from a total of 49 224 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Furosemide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Furosemide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	200	0	201 884
Type C	0	74	0	235 993

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The substance/substance group *Furosemide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 91.8919 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20944	20944	0.00	375.75
21819	20944	11.31	372.08
23940	20944	10.08	374.24
25044	20944	4.36	380.19
26607	20944	7.97	383.26
26977	20944	8.51	385.65

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Fusidic acid**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20780-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Fusidic acid; Acidum fusidicum

Special notes

When selecting the *Fusidic acid* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Fusidic acid	5	3	37

Second-stage model

For differentiation of the substance/substance group *Fusidic acid* the following second-stage model is used:

- Submodel 05

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Fusidic acid* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	91.90	–
⋮	⋮	⋮
Povidone	>50	78.18
Povidone iodine	>50	89.05
Progesterone	>50	115.66
Spironolactone	>50	122.16
Testosterone propionate	>50	176.82
Ubidecarenone	>50	223.28

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Fusidic acid* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Fusidic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Fusidic acid	12G04-N01	20780	40	1401162
Fagron	Fusidic acid	13L13-B01-289513	21733	60	20140113
Fagron	Fusidic acid	14E01-B08-299791	21897	60	20140605
Fagron	Fusidic acid	20J21-F02-375395	25493	40	2104173
Fagron	Fusidic acid	23K21-B01-233624	27045	40	20231206

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 240 spectra of 5 reference samples from the substance/substance group *Fusidic acid*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 722 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 5 reference samples from the substance/substance group *Fusidic acid*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Fusidic acid	15I10-B02-322112	23069	40
Fagron	Fusidic acid	17J06-B02-343675	23943	40
Fagron	Fusidic acid	22E23-B03-220268	26296	40
Fagron	Fusidic acid	22E23-B03-220268	26296SI	20
Fagron	Fusidic acid	23K21-B01-233624	27045SI†	20

- 201 924 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 55 spectra from 25 *Apo-Ident* customers from 40 batches from the substance/substance group *Fusidic acid*.

- Among them are spectra of independent samples from 37 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Fusidic acid	21K17-B02-216070	1
	Fusidic acid	22E23-B03-220268	1
Caelo	Fusidic acid	21E12-F08-378510	1
Ebert 24.08.16	Fusidic acid	1510-B02_319452	1
Fagron	Fusidic acid	1119I-03682	1
Fagron	Fusidic acid	116E-03682	1
Fagron	Fusidic acid	12B23-N03	1
Fagron	Fusidic acid	12G04-No1	1
Fagron	Fusidic acid	13A07-N10	2
Fagron	Fusidic acid	13H19-N05	1
Fagron	Fusidic acid	13L13-B01	1
Fagron	Fusidic acid	13L13-B01-289513	3
Fagron	Fusidic acid	13L13-B01-289514	1
Fagron	Fusidic acid	14E01-B08-299791	3
Fagron	Fusidic acid	15/10-b02	2
Fagron	Fusidic acid	15/10-B02-314192	1
Fagron	Fusidic acid	15/10-B02-319452	1
Fagron	Fusidic acid	1510-B02_319231	1
Fagron	Fusidic acid	15I10-B02	1
Fagron	Fusidic acid	15I10B02-319231	1
Fagron	Fusidic acid	15I10-B02-326182	1
Fagron	Fusidic acid	17G06-B99-337953	1
Fagron	Fusidic acid	17J06-B02-343677	1
Fagron	Fusidic acid	17J06-B02-345542	1
Fagron	Fusidic acid	17J06-B02-345885	1
Fagron	Fusidic acid	17J06-B02-355108	1
Fagron	Fusidic acid	20J21-F01-375395	1
Fagron	Fusidic acid	20J21-F02-375395	1
Fagron	Fusidic acid	20J21-F02-375397	2
Fagron	Fusidic acid	21D12-B08-213764	2
Fagron	Fusidic acid	21E12-F08	1
Fagron	Fusidic acid	21E12-F08-378510	2
Fagron	Fusidic acid	21H13-B05-213845	3
Fagron	Fusidic acid	21H13-BO5-213845	1
Fagron	Fusidic acid	21K17-B02-216069	3
Fagron	Fusidic acid	318A-03682	1
Fagron	Fusidic acid	4113U-07034	1
Fagron	Fusidic acid	FS655	1
Noweda	Fusidic acid	17J06-B02-349947	1
Phoenix/Cealo	Fusidic acid	701714-0003/0918A-07	1
Phönix	Fusidic acid	F03-3691901	1
Tagron	Fusidic acid	17J06-B02-355108	1

- 236 012 spectra from 1515 *Apo-Ident* customers from a total of 49 218 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Fusidic acid* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Fusidic acid* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	240	0	152 722
Type B	0	160	0	201 924
Type C	0	55	0	236 012

The substance/substance group *Fusidic acid* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 89.0909 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20780	20780	0.00	121.17
21733	20780	7.12	123.10
21897	20780	32.12	121.21
25493	25493	0.00	126.48
27045	20780	32.46	133.95

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Gabapentin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10005490-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gabapentin; Gabapentinum

Special notes

When selecting the *Gabapentin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Gabapentin	3	2	4

Second-stage model

For differentiation of the substance/substance group *Gabapentin* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Gabapentin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Tranexamic acid	76.20	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Gabapentin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Gabapentin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Gabapentin	21G13-B17-215252	26079	40	20220329
Hikal Ltd.	Gabapentin	G71010620/077	25833	50	2203054
Hikal Ltd.	Gabapentin	B71010621/105	25898	50	20211111

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 140 spectra of 3 reference samples from the substance/substance group *Gabapentin*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 152 822 spectra from a total of 2839 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 7 reference samples from the substance/substance group *Gabapentin*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Gabapentin	22H02-B04-228420	26614	40
MEDICHEM S.A.	Gabapentin	A-180101	25837	50
Fagron	Gabapentin	21G13-B17-215252	26079SI†	40
Fagron	Gabapentin	22H02-B04-228420	26614SI	20
Hikal Ltd.	Gabapentin	G71010620/077	25833SI†	10
Hikal Ltd.	Gabapentin	B71010621/105	25898SI†	10
MEDICHEM S.A.	Gabapentin	A-180101	25837SI	10

- 201 904 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 9 spectra from 3 *Apo-Ident* customers from 4 batches from the substance/substance group *Gabapentin*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Gabapentin	22H02-B04-228420	3
	Gabapentin	B04-2284200	4
Fagron	Gabapentin	21G13-B17-2152502	1
INRESA/INRESA	Gabapentin	B71010621/409	1

- 236 058 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Gabapentin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gabapentin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	140	0	152 822
Type B	0	180	0	201 904
Type C	0	9	0	236 058

The substance/substance group *Gabapentin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.7143 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25833	25833	0.00	144.97
25898	25833	15.75	152.28
26079	25833	16.84	151.86

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Galactose**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20326-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Galactose; Galactosum

Special notes

When selecting the *Galactose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Galactose	4	3	27

Second-stage model

For differentiation of the substance/substance group *Galactose* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Galactose* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	68.41	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Galactose* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Galactose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Galactose	13I13-B40-287993	21762	60	AR-15-FG-008936-01
Fagron	Galactose	14H05-B09-310972	22259	60	20140818
Fagron	Galactose	18F14-B02-355816	25179	40	20181212
Fagron	Galactose	23H08-F01-385354	27032	40	20231009
Fagron	Galactose	23H08-F01-385354	27032SI	20	20231009

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 220 spectra of 5 reference samples from the substance/substance group *Galactose*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 742 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 5 reference samples from the substance/substance group *Galactose*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Galactose	15G13-B04-320810	23106	40
Fagron	Galactose	19G12-F50-373175	25443	40
Fagron	Galactose	24H01-B08-001699	27422	40
Fagron	Galactose	15G13-B04-320810	23595	40
Fagron	Galactose	24H01-B08-001699	27422SI	20

- 201 904 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 39 spectra from 5 *Apo-Ident* customers from 28 batches from the substance/substance group *Galactose*.
- Among them are spectra of independent samples from 27 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Applichem	Galactose	2L009814	1
Fagron	Galactose	16G22-B01-329906	1
Falcento	Galactose	10440003	1
Falcento	Galactose	12223PF4	2
Falcento	Galactose	1223PF4	3
Falcento	Galactose	122PF4	1
Falcento	Galactose	13223PF4	1
Falcento	Galactose	2014	1
Falcento	Galactose	2223PF4	3
Falcento	Galactose	222PF4	1
Falcento	Galactose	233619PF5	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
falcento	Galactose	322619PF5	1
Falcento	Galactose	48223PF2	1
Falcento	Galactose	5223PF4	3
Falcento	Galactose	72619PF7	1
Falcento	Galactose	82619PF64743/16	1
Falcento	Galactose	82619PF7	1
Falcento	Galactose	92619PF64744/16	1
inalco	Galactose	212619PF5	1
inalco	Galactose	32619PF8	1
inalco	Galactose	42619PF4	1
Phönix 04.03.2014	Galactose		1
Phönix	Galactose	39223PF3	1
Unisan	Galactose	382619PF5	1
Unisan	Galactose	432619PF5	1
Unisan	Galactose	442619PF5	1
vwr chemicals	Galactose	1F012304	1
VWR	Galactose	9Y013597	5

- 236 028 spectra from 1515 *Apo-Ident* customers from a total of 49 230 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Galactose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Galactose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	220	0	152 742
Type B	0	180	0	201 904
Type C	0	39	0	236 028

The substance/substance group *Galactose* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 84.6154 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21762	21762	0.00	190.13
22259	21762	18.46	178.48
25179	21762	15.17	186.12
27032	21762	19.20	190.07

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Gelatine, white**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20206-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gelatine, white; Gelatina alba

Special notes

When selecting the *Gelatine, white* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Gelatine, white	3	3	34

Second-stage model

For differentiation of the substance/substance group *Gelatine, white* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Gelatine, white* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	42.29	32.65
Cyanocobalamin	74.37	37.64
⋮	⋮	⋮
Colistin sulfate	>50	22.69
Bacitracin	>50	24.36
Amphotericin B	>50	44.52
Nystatin	>50	56.87
Calcium pantothenate	>50	59.53
Methylcobalamin	>50	70.81
Riboflavin	>50	75.37
alpha-tocopheryl acetate dry concentrate	>50	81.43
Triamcinolone	>50	93.10
Calcium glycerophosphate	>50	93.55
Carmellose sodium	>50	101.48
Selenium yeast	>50	108.84
Hyoscine hydrobromide	>50	112.63
Estradiol hemihydrate	>50	123.13
Tosylchloramide sodium	>50	134.02
Estriol	>50	141.15
SyrSpend® SF Alka	>50	150.01
Rice starch	>50	163.00
Oxalic acid	>50	169.23
SyrSpend® SF pH4 neo (Maize starch)	>50	181.51
SyrSpend® SF pH4	>50	195.23
Acacia, dried dispersion	>50	235.94
Corn starch	>50	237.91
Potato starch	>50	290.73
Wheat starch	>50	305.82
Maltodextrin	>50	318.99
Fructose	>50	326.18

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Gelatine, white* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Gelatine, white*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Gelatine, white	11334025	20898	40	20111214
Caelo	Gelatine, white	15320504	22499	40	AR-16-FG-014461-01
Caelo	Gelatine, white	15320504	22582	45	AR-16-FG-011564-01
Caelo	Gelatine, white	20000813	25289	40	20200417*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 165 spectra of 4 reference samples from the substance/substance group *Gelatine, white*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 152 797 spectra from a total of 2839 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Gelatine, white*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Gelatine, white	172772	23792	40
Caelo	Gelatine, white	154419	23793	40
Caelo	Gelatine, white	23002360	26943	40
Caelo	Gelatine, white	23002360	26943SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 944 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 49 spectra from 32 *Apo-Ident* customers from 35 batches from the substance/substance group *Gelatine, white*.

- Among them are spectra of independent samples from 34 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Gelatine, white	2003763018	1
Caealo/Phoenix	Gelatine, white	20003763003	2
Caelo	Gelatine, white	11019308	1
Caelo	Gelatine, white	11334020	1
Caelo	Gelatine, white	11334025	4
Caelo	Gelatine, white	12354401	1
Caelo	Gelatine, white	12354507	3
Caelo	Gelatine, white	14130901	2
Caelo	Gelatine, white	14130912	1
Caelo	Gelatine, white	15084801	1
Caelo	Gelatine, white	15084806	1
Caelo	Gelatine, white	15320502	2
Caelo	Gelatine, white	15441902	1
Caelo	Gelatine, white	1544191916	1
Caelo	Gelatine, white	15441922	1
Caelo	Gelatine, white	17277207	1
Caelo	Gelatine, white	17277210	1
Caelo	Gelatine, white	190907004	1
Caelo	Gelatine, white	19090702	1
Caelo	Gelatine, white	19090706	1
Caelo	Gelatine, white	20003763001	1
Caelo	Gelatine, white	20003763004	1
Caelo	Gelatine, white	20003763006	1
Caelo	Gelatine, white	20003763009	2
Caelo	Gelatine, white	4110I-01578	1
Caelo	Gelatine, white	8031701	1
Caelo	Gelatine, white	8051811	1
Caesar & Loretz GmbH...	Gelatine, white	20003763002	1
Caesar & Loretz GmbH...	Gelatine, white	190907004	1
Caesar & Loretz GmbH	Gelatine, white	17277208	1
Caesar & Loretz GmbH	Gelatine, white	17277213	1
Caesar & Loretz GmbH	Gelatine, white	190907001	1
Caesar & Loretz GmbH	Gelatine, white	190907002	3
canea Pharma/noweda	Gelatine, white	GR1617	1
EuRho / 20	Gelatine, white	1106021-01	1
Euro OTC	Gelatine, white	1106021-01	2
ROHA	Gelatine, white	140110	1

- 236 018 spectra from 1515 *Apo-Ident* customers from a total of 49 224 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are docu-

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

mented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Gelatine, white* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gelatine, white* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	165	0	152 797
Type B	0	140	0	201 944
Type C	0	49	0	236 018

The substance/substance group *Gelatine, white* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.3636 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 87.7551 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20898	22582	9.12	95.36
22499	22499	0.00	94.01
22582	22582	0.00	90.86
25289	25289	0.00	97.72

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Gentamicin sulfate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20640-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gentamicin sulfate; Gentamicin sulphate; Gentamicini sulfas

Special notes

When selecting the *Gentamicin sulfate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Gentamicin sulfate	17	9	358

Second-stage model

For differentiation of the substance/substance group *Gentamicin sulfate* the following second-stage model is used:

- Submodel 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Gentamicin sulfate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	46.53	–
Polymyxin B sulfate	48.85	–
Riboflavin sodium phosphate hydrate	51.77	32.87
⋮	⋮	⋮
Mg-Ca-K colamine phosphate	>50	36.72
Magnesium citrate	>50	62.40
Neomycin sulfate	>50	74.18
Carbomers	>50	77.76
Zinc gluconate	>50	103.21
Tobramycin sulfate	>50	126.45
Sodium tetraborate	>50	262.45
Finasteride	>50	1065.07

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Gentamicin sulfate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Gentamicin sulfate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Gentamicin sulfate	13205003	21580	60	20130723
Caelo	Gentamicin sulfate	14353504	22604	40	20150119
Caelo	Gentamicin sulfate	192564	25201	40	20191218*
Caelo	Gentamicin sulfate	192564	25201SI	40	20191218*
Caelo	Gentamicin sulfate	20003226	25638	40	20201029*
Caelo	Gentamicin sulfate	20003226	25638SI	40	20201029*
Euro OTC	Gentamicin sulfate	1305047-01	21081	30	20130919
Euro OTC	Gentamicin sulfate	1305047-03	21582	60	1411076
Euro OTC	Gentamicin sulfate	1305047-03	21697	45	AR-15-FG-012403-01
Euro OTC	Gentamicin sulfate	1506016	21837	60	0000010321

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Gentamicin sulfate	1610036	22857	40	20161124*
Euro OTC	Gentamicin sulfate	1610036-01	23782	40	1804343
Euro OTC	Gentamicin sulfate	1711025	23882	40	20171206*
Euro OTC	Gentamicin sulfate	1711025	23882SI	40	20171206*
Euro OTC	Gentamicin sulfate	1907036	24866	40	20190823*
Euro OTC	Gentamicin sulfate	2003058	25252	40	20200603*
Euro OTC	Gentamicin sulfate	2003058	25252SI	40	20200603*
Fagron	Gentamicin sulfate	12B21-N02	20661	40	1411075
Fagron	Gentamicin sulfate	13I19-B05-286565	21578	60	20121214
Fagron	Gentamicin sulfate	14E08-B03-294848	21684	60	20140616
Fagron	Gentamicin sulfate	16B29-B01-328731	23210	40	20160411
Fagron	Gentamicin sulfate	19G17-B05-193462	25180	40	20190805
Fagron	Gentamicin sulfate	19G17-B05-193462	25180SI	40	20190805

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1015 spectra of 23 reference samples from the substance/substance group *Gentamicin sulfate*. These samples are listed above in the *calibration samples* section. The reference samples come from 17 different batches.

- 151 947 spectra from a total of 2825 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 950 spectra of 21 reference samples from the substance/substance group *Gentamicin sulfate*.

- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Gentamicin sulfate	170996	23335	40
Caelo	Gentamicin sulfate	183001	24357	40
Caelo	Gentamicin sulfate	23001024	27128	40
Euro OTC	Gentamicin sulfate	1604054	22568	40
Euro OTC	Gentamicin sulfate	1808013	24300	40
Euro OTC	Gentamicin sulfate	2107013	25825	50
Euro OTC	Gentamicin sulfate	2203032	26083	40
Euro OTC	Gentamicin sulfate	2210010	26434	40
Fagron	Gentamicin sulfate	22C17-B10-218675	26181	40
Caelo	Gentamicin sulfate	13205003	21580SI†	60
Caelo	Gentamicin sulfate	183001	24357SI	40
Caelo	Gentamicin sulfate	23001024	27128SI	40
Euro OTC	Gentamicin sulfate	1506016	21837SI†	60
Euro OTC	Gentamicin sulfate	1808013	24300SI	40
Euro OTC	Gentamicin sulfate	1907036	24866SI†	40
Euro OTC	Gentamicin sulfate	2107013	25825SI	50
Euro OTC	Gentamicin sulfate	2203032	26083SI	50
Euro OTC	Gentamicin sulfate	2210010	26434SI	40
Fagron	Gentamicin sulfate	13I19-B05-286565	21578SI†	60
Fagron	Gentamicin sulfate	14E08-B03-294848	21684SI†	60
Fagron	Gentamicin sulfate	22C17-B10-218675	26181SI	40

- 201 134 spectra from a total of 4031 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2537 spectra from 961 *Apo-Ident* customers from 384 batches from the substance/substance group *Gentamicin sulfate*.

- Among them are spectra of independent samples from 355 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Gentamicin sulfate	1610038-01	1
	Gentamicin sulfate	20004483009	1
	Gentamicin sulfate	20004483012	1
	Gentamicin sulfate	2107013-02	2
	Gentamicin sulfate	210920013	1
	Gentamicin sulfate	2200075012	1
	Gentamicin sulfate	22000754001	3
	Gentamicin sulfate	22000754003	8
	Gentamicin sulfate	22000754006	4
	Gentamicin sulfate	22000754011	2
	Gentamicin sulfate	22000754012	6
	Gentamicin sulfate	22000754013	5
	Gentamicin sulfate	2203032-01	3
	Gentamicin sulfate	2210010-01	4

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Gentamicin sulfate	2210010-02	2
	Gentamicin sulfate	2210010-03	1
	Gentamicin sulfate	22C17-B010-223074	1
	Gentamicin sulfate	22C17-B10	1
	Gentamicin sulfate	22c17-b10-223074	1
	Gentamicin sulfate	22F28-B02-233049	1
	Gentamicin sulfate	22I14-B01-227901	1
	Gentamicin sulfate	23001024001	3
	Gentamicin sulfate	23001024004	9
	Gentamicin sulfate	23001024005	1
	Gentamicin sulfate	23G05-B07-236824	1
AHD /Pharmachem Pößneck	Gentamicin sulfate	1506016-02	1
AHD 29.10.14 EK6,12	Gentamicin sulfate	13205004	1
AHD Lamotte GmbH	Gentamicin sulfate	1604054-02	1
AHD	Gentamicin sulfate	13205005	2
AHD	Gentamicin sulfate	22000754003	1
AHD	Gentamicin sulfate	22000754012	1
AHD	Gentamicin sulfate	22000754013	1
AHD	Gentamicin sulfate	23001024001	1
ALH	Gentamicin sulfate	15258813	1
ALH	Gentamicin sulfate	15258816	1
Alliance Healtcare	Gentamicin sulfate	2003058-01	3
Alliance Healthcare	Gentamicin sulfate	12G04-N16	1
Anzag	Gentamicin sulfate	12146602	1
Anzag	Gentamicin sulfate	1305047-03	1
Anzag	Gentamicin sulfate	1407024-01	1
Anzag	Gentamicin sulfate	17K16-B09-343323	1
Apo Ident/ Noweda	Gentamicin sulfate	1711025	1
Apotheke	Gentamicin sulfate	2003058-02	2
Audor Pharma	Gentamicin sulfate	1604054-01	1
Bombastus	Gentamicin sulfate	1205021-01	1
Bombastus	Gentamicin sulfate	13024-N05	1
Bombastus	Gentamicin sulfate	17358616	1
Bombastus	Gentamicin sulfate	700175	1
Caelo	Gentamicin sulfate		3
Caelo	Gentamicin sulfate	10(18300112)	1
Caelo	Gentamicin sulfate	100017814	1
Caelo	Gentamicin sulfate	1106016-01	1
Caelo	Gentamicin sulfate	1106016-03	1
Caelo	Gentamicin sulfate	11113303	2
Caelo	Gentamicin sulfate	11113304	1
Caelo	Gentamicin sulfate	11113308	4
Caelo	Gentamicin sulfate	115258818	1
Caelo	Gentamicin sulfate	12011801	1
Caelo	Gentamicin sulfate	1205021-01	1
Caelo	Gentamicin sulfate	1205021-02	2
Caelo	Gentamicin sulfate	12146602	7
Caelo	Gentamicin sulfate	12146604	6
Caelo	Gentamicin sulfate	12146605	4
Caelo	Gentamicin sulfate	12146611	11
Caelo	Gentamicin sulfate	12146612	2
Caelo	Gentamicin sulfate	12163204	4
Caelo	Gentamicin sulfate	12163206	1
Caelo	Gentamicin sulfate	12163207	3
Caelo	Gentamicin sulfate	12163209	1
Caelo	Gentamicin sulfate	12258813	1
Caelo	Gentamicin sulfate	1260417	1
Caelo	Gentamicin sulfate	12G04-N16	2
Caelo	Gentamicin sulfate	130205005	1
Caelo	Gentamicin sulfate	1305047-03	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Gentamicin sulfate	1305047-03(2mal)	1
Caelo	Gentamicin sulfate	13091207	1
Caelo	Gentamicin sulfate	13189602	5
Caelo	Gentamicin sulfate	13189603	3
Caelo	Gentamicin sulfate	13189606	6
Caelo	Gentamicin sulfate	13189607	11
Caelo	Gentamicin sulfate	13189608	2
Caelo	Gentamicin sulfate	13189611	10
Caelo	Gentamicin sulfate	13189612	13
Caelo	Gentamicin sulfate	13189613	1
Caelo	Gentamicin sulfate	13189614	2
Caelo	Gentamicin sulfate	13205003	10
Caelo	Gentamicin sulfate	13205004	2
Caelo	Gentamicin sulfate	13205005	17
Caelo	Gentamicin sulfate	13205006	6
Caelo	Gentamicin sulfate	13205007	2
Caelo	Gentamicin sulfate	13D24-N05	1
Caelo	Gentamicin sulfate	13I19-B05-286565	1
Caelo	Gentamicin sulfate	14081307	1
Caelo	Gentamicin sulfate	1435303	2
Caelo	Gentamicin sulfate	143533504	1
Caelo	Gentamicin sulfate	143535	1
Caelo	Gentamicin sulfate	14353502	3
Caelo	Gentamicin sulfate	14353503	13
Caelo	Gentamicin sulfate	14353504	12
Caelo	Gentamicin sulfate	14353505	3
Caelo	Gentamicin sulfate	14E08-B03-294841	1
Caelo	Gentamicin sulfate	14K28-B06-303636	1
Caelo	Gentamicin sulfate	14K28-B06-303646	3
Caelo	Gentamicin sulfate	150320G	1
Caelo	Gentamicin sulfate	1506016-01	2
Caelo	Gentamicin sulfate	1506016-02	2
Caelo	Gentamicin sulfate	15128818	1
Caelo	Gentamicin sulfate	15226501	20
Caelo	Gentamicin sulfate	15226502	15
Caelo	Gentamicin sulfate	1522650217099604	1
Caelo	Gentamicin sulfate	15226508	2
Caelo	Gentamicin sulfate	15226513	1
Caelo	Gentamicin sulfate	15226514	5
Caelo	Gentamicin sulfate	15226517	1
Caelo	Gentamicin sulfate	15226518	9
Caelo	Gentamicin sulfate	15258802	15
Caelo	Gentamicin sulfate	15258803	17
Caelo	Gentamicin sulfate	15258805	2
Caelo	Gentamicin sulfate	15258808	10
Caelo	Gentamicin sulfate	15258809	1
Caelo	Gentamicin sulfate	15258810	18
Caelo	Gentamicin sulfate	15258813	14
Caelo	Gentamicin sulfate	15258815	3
Caelo	Gentamicin sulfate	15258816	16
Caelo	Gentamicin sulfate	15258818	33
Caelo	Gentamicin sulfate	15258819	6
Caelo	Gentamicin sulfate	15258825	2
Caelo	Gentamicin sulfate	1528802	1
Caelo	Gentamicin sulfate	1528818	1
Caelo	Gentamicin sulfate	15B03-B07-309482	1
Caelo	Gentamicin sulfate	1604054-01	3
Caelo	Gentamicin sulfate	1604054-02	1
Caelo	Gentamicin sulfate	1604054-03	1
Caelo	Gentamicin sulfate	1610036-01	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Gentamicin sulfate	161003602	1
Caelo	Gentamicin sulfate	16119302	1
Caelo	Gentamicin sulfate	16b29-b01-328731	1
Caelo	Gentamicin sulfate	16B29-B01-328731	1
Caelo	Gentamicin sulfate	17081502	1
Caelo	Gentamicin sulfate	1709601	1
Caelo	Gentamicin sulfate	17099601	3
Caelo	Gentamicin sulfate	17099603	28
Caelo	Gentamicin sulfate	17099604	19
Caelo	Gentamicin sulfate	17099606	20
Caelo	Gentamicin sulfate	17099606-20180404Ma1	1
Caelo	Gentamicin sulfate	17099608	24
Caelo	Gentamicin sulfate	1710I-01582	1
Caelo	Gentamicin sulfate	1711025	1
Caelo	Gentamicin sulfate	1711025-01	2
Caelo	Gentamicin sulfate	1711025-02	4
Caelo	Gentamicin sulfate	17332419	1
Caelo	Gentamicin sulfate	17358603	35
Caelo	Gentamicin sulfate	17358604	12
Caelo	Gentamicin sulfate	17358607	2
Caelo	Gentamicin sulfate	17358609	39
Caelo	Gentamicin sulfate	17358609P-180201-2	1
Caelo	Gentamicin sulfate	17358610	11
Caelo	Gentamicin sulfate	17358616	37
Caelo	Gentamicin sulfate	17358618	14
Caelo	Gentamicin sulfate	17358619	1
Caelo	Gentamicin sulfate	17358623	1
Caelo	Gentamicin sulfate	17358909	1
Caelo	Gentamicin sulfate	1800104	1
Caelo	Gentamicin sulfate	18041804	1
Caelo	Gentamicin sulfate	180801301	2
Caelo	Gentamicin sulfate	1808013-01	2
Caelo	Gentamicin sulfate	183001001	1
Caelo	Gentamicin sulfate	183001002	1
Caelo	Gentamicin sulfate	183001004	20
Caelo	Gentamicin sulfate	18300103	7
Caelo	Gentamicin sulfate	18300104	26
Caelo	Gentamicin sulfate	18300108	12
Caelo	Gentamicin sulfate	18300109	40
Caelo	Gentamicin sulfate	183001112	1
Caelo	Gentamicin sulfate	18300112	28
Caelo	Gentamicin sulfate	18300113	27
Caelo	Gentamicin sulfate	18300114	9
Caelo	Gentamicin sulfate	18399104	1
Caelo	Gentamicin sulfate	18C12-B02-349026	1
Caelo	Gentamicin sulfate	18G06-B09-354797	1
Caelo	Gentamicin sulfate	18Go6-351916	1
Caelo	Gentamicin sulfate	190703601	1
Caelo	Gentamicin sulfate	1907036-01	1
Caelo	Gentamicin sulfate	192564002	29
Caelo	Gentamicin sulfate	192564003	19
Caelo	Gentamicin sulfate	192564004	2
Caelo	Gentamicin sulfate	192564008	1
Caelo	Gentamicin sulfate	192564009	7
Caelo	Gentamicin sulfate	192564010	21
Caelo	Gentamicin sulfate	19256402	1
Caelo	Gentamicin sulfate	19300109	1
Caelo	Gentamicin sulfate	19300113	1
Caelo	Gentamicin sulfate	200004483010	1
Caelo	Gentamicin sulfate	20004482002	21

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Gentamicin sulfate	20004482004	6
Caelo	Gentamicin sulfate	20004483	1
Caelo	Gentamicin sulfate	20004483001	37
Caelo	Gentamicin sulfate	200044830014	1
Caelo	Gentamicin sulfate	20004483005	12
Caelo	Gentamicin sulfate	20004483006	1
Caelo	Gentamicin sulfate	20004483007	15
Caelo	Gentamicin sulfate	20004483008	1
Caelo	Gentamicin sulfate	20004483009	8
Caelo	Gentamicin sulfate	20004483010	22
Caelo	Gentamicin sulfate	20004483011	1
Caelo	Gentamicin sulfate	20004483012	1
Caelo	Gentamicin sulfate	20004483013	4
Caelo	Gentamicin sulfate	20004483014	21
Caelo	Gentamicin sulfate	2000448310	1
Caelo	Gentamicin sulfate	2003058-02	1
Caelo	Gentamicin sulfate	2004483009	1
Caelo	Gentamicin sulfate	2004483014	2
Caelo	Gentamicin sulfate	20161102-4	1
Caelo	Gentamicin sulfate	20170829/1	1
Caelo	Gentamicin sulfate	2200075400	1
Caelo	Gentamicin sulfate	22000754001	16
Caelo	Gentamicin sulfate	22000754003	11
Caelo	Gentamicin sulfate	22000754006	11
Caelo	Gentamicin sulfate	22000754012	1
Caelo	Gentamicin sulfate	2200754001	1
Caelo	Gentamicin sulfate	23012015E	1
Caelo	Gentamicin sulfate	2794	1
Caelo	Gentamicin sulfate	31032014E	1
Caelo	Gentamicin sulfate	3110806	1
Caelo	Gentamicin sulfate	312012	1
Caelo	Gentamicin sulfate	3265	1
Caelo	Gentamicin sulfate	3714I-01582	1
Caelo	Gentamicin sulfate	4563125	1
Caelo	Gentamicin sulfate	6082013C	1
Caelo	Gentamicin sulfate	7011505	1
Caelo	Gentamicin sulfate	73402189	1
Caelo	Gentamicin sulfate	8702	1
Caelo	Gentamicin sulfate	B18-1955204	1
Caelo	Gentamicin sulfate	FG1503073	1
Caelo	Gentamicin sulfate	FG1603072	1
Caeol/ Noweda	Gentamicin sulfate	15258803	2
Caesar & Loretz GmbH...	Gentamicin sulfate	18300113	1
Caesar & Loretz GmbH...	Gentamicin sulfate	192564010	1
Caesar & Loretz GmbH...	Gentamicin sulfate	17358603	1
Caesar & Loretz GmbH...	Gentamicin sulfate	183001004	1
Caesar & Loretz GmbH...	Gentamicin sulfate	17358609	1
Caesar & Loretz GmbH...	Gentamicin sulfate	20004483005	1
Caesar & Loretz GmbH...	Gentamicin sulfate	18300109	1
Caesar & Loretz GmbH...	Gentamicin sulfate	20004482002	1
Caesar & Loretz GmbH/AEP	Gentamicin sulfate	20004483010	1
Caesar & Loretz GmbH/Gehe	Gentamicin sulfate	20004483014	1
Caesar & Loretz GmbH...	Gentamicin sulfate	20004483010	1
Caesar & Loretz GmbH...	Gentamicin sulfate	20004482004	1
Caesar & Loretz GmbH...	Gentamicin sulfate	20004483009	1
Caesar & Loretz GmbH/Kehr	Gentamicin sulfate	18300112	1
Caesar & Loretz GmbH/Kehr	Gentamicin sulfate	192564010	1
Caesar & Loretz GmbH...	Gentamicin sulfate	192564010	1
Caesar & Loretz GmbH...	Gentamicin sulfate	18300104	1
Caesar & Loretz GmbH...	Gentamicin sulfate	18300113	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Gentamicin sulfate	18300104	1
Caesar & Loretz GmbH...	Gentamicin sulfate	18300114	1
Caesar & Loretz GmbH...	Gentamicin sulfate	192564002	1
Caesar & Loretz GmbH...	Gentamicin sulfate	192564008	1
Caesar & Loretz GmbH...	Gentamicin sulfate	20004483005	1
Caesar & Loretz GmbH...	Gentamicin sulfate	20004483013	1
Caesar & Loretz GmbH/Otto	Gentamicin sulfate	192564003	1
Caesar & Loretz GmbH/Ph	Gentamicin sulfate	183001004	1
Caesar & Loretz GmbH...	Gentamicin sulfate	192564010	1
Caesar & Loretz GmbH...	Gentamicin sulfate	18300112	1
Caesar & Loretz GmbH...	Gentamicin sulfate	18300113	1
Caesar & Loretz GmbH...	Gentamicin sulfate	20004483001	1
Caesar & Loretz GmbH...	Gentamicin sulfate	20004483007	1
Caesar & Loretz GmbH...	Gentamicin sulfate	22000754003	1
Caesar & Loretz GmbH...	Gentamicin sulfate	18300108	1
Caesar & Loretz GmbH...	Gentamicin sulfate	192564002	2
Caesar & Loretz GmbH...	Gentamicin sulfate	183001004	1
Caesar & Loretz GmbH...	Gentamicin sulfate	192564010	2
Caesar & Loretz GmbH...	Gentamicin sulfate	20004482002	3
Caesar & Loretz GmbH...	Gentamicin sulfate	20004483001	3
Caesar & Loretz GmbH...	Gentamicin sulfate	20004483005	1
Caesar & Loretz GmbH...	Gentamicin sulfate	20004483010	1
Caesar & Loretz GmbH...	Gentamicin sulfate	20004483014	1
Caesar & Loretz GmbH	Gentamicin sulfate	14353503	1
Caesar & Loretz GmbH	Gentamicin sulfate	17099604	1
Caesar & Loretz GmbH	Gentamicin sulfate	17358607	1
Caesar & Loretz GmbH	Gentamicin sulfate	17358609	1
Caesar & Loretz GmbH	Gentamicin sulfate	17358610	1
Caesar & Loretz GmbH	Gentamicin sulfate	17358616	5
Caesar & Loretz GmbH	Gentamicin sulfate	17358618	3
Caesar & Loretz GmbH	Gentamicin sulfate	17358619	1
Caesar & Loretz GmbH	Gentamicin sulfate	183001002	4
Caesar & Loretz GmbH	Gentamicin sulfate	183001004	14
Caesar & Loretz GmbH	Gentamicin sulfate	18300103	1
Caesar & Loretz GmbH	Gentamicin sulfate	18300104	11
Caesar & Loretz GmbH	Gentamicin sulfate	18300108	3
Caesar & Loretz GmbH	Gentamicin sulfate	18300109	6
Caesar & Loretz GmbH	Gentamicin sulfate	18300110	2
Caesar & Loretz GmbH	Gentamicin sulfate	18300112	10
Caesar & Loretz GmbH	Gentamicin sulfate	18300113	7
Caesar & Loretz GmbH	Gentamicin sulfate	18300114	5
Caesar & Loretz GmbH	Gentamicin sulfate	192564002	8
Caesar & Loretz GmbH	Gentamicin sulfate	192564003	3
Caesar & Loretz GmbH	Gentamicin sulfate	192564006	1
Caesar & Loretz GmbH	Gentamicin sulfate	192564008	2
Caesar & Loretz GmbH	Gentamicin sulfate	192564009	4
Caesar & Loretz GmbH	Gentamicin sulfate	192564010	10
Caesar & Loretz GmbH	Gentamicin sulfate	19256410	1
Caesar & Loretz GmbH	Gentamicin sulfate	20004482002	6
Caesar & Loretz GmbH	Gentamicin sulfate	20004482004	5
Caesar & Loretz GmbH	Gentamicin sulfate	20004483001	11
Caesar & Loretz GmbH	Gentamicin sulfate	20004483002	1
Caesar & Loretz GmbH	Gentamicin sulfate	20004483005	3
Caesar & Loretz GmbH	Gentamicin sulfate	20004483007	4
Caesar & Loretz GmbH	Gentamicin sulfate	20004483009	5
Caesar & Loretz GmbH	Gentamicin sulfate	20004483010	13
Caesar & Loretz GmbH	Gentamicin sulfate	20004483012	3
Caesar & Loretz GmbH	Gentamicin sulfate	20004483013	7
Caesar & Loretz GmbH	Gentamicin sulfate	20004483014	6
Caesar & Loretz GmbH	Gentamicin sulfate	20004486010	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Gentamicin sulfate	22000754001	3
Caesar & Loretz GmbH	Gentamicin sulfate	22000754003	7
Caesar & Loretz GmbH	Gentamicin sulfate	22000754006	6
Caesar & Loretz	Gentamicin sulfate	17358603	1
Caesar & Loretz	Gentamicin sulfate	20004483007	1
Caesar / Ebert	Gentamicin sulfate	15258818	1
Caesar&Loretz GmbH,2...	Gentamicin sulfate	15258802	1
Caesar&Loretz GmbH	Gentamicin sulfate	15226501	1
Caesar&Loretz GmbH	Gentamicin sulfate	1907036-01	1
Caleo/ Noweda	Gentamicin sulfate	17099606	1
Cealo / Anzag	Gentamicin sulfate	211108(20004483007)	1
Cealo	Gentamicin sulfate		1
Celo/Jenne	Gentamicin sulfate	17099603	1
CL/Gehe	Gentamicin sulfate	17358616	1
Delta Apotheke	Gentamicin sulfate	17358604	2
Ebert & Jacobi	Gentamicin sulfate	1506016-01	1
EuRho / Gehe	Gentamicin sulfate	2003058-02	2
EuRho / Phönix	Gentamicin sulfate	1610036-02	1
Eurho AHD 20.11.19 E...	Gentamicin sulfate	1808013-02	1
Eurho Phönix	Gentamicin sulfate	2107013-2	1
EuRho/Gehe	Gentamicin sulfate	2003058-01	1
EuRho/Gehe	Gentamicin sulfate	2003058-02	2
EuRho/Krieger	Gentamicin sulfate	1711025-02	1
Eurho/Noweda	Gentamicin sulfate	1604054-02	1
EuRho/Noweda	Gentamicin sulfate	1907036-01	2
EuRho/Phoenix	Gentamicin sulfate	1808013-02	1
Eurho/Phönix	Gentamicin sulfate	200305802	1
EuRho/Phönix	Gentamicin sulfate	2003058-02	1
EuRho	Gentamicin sulfate	1106016-03	1
EuRho	Gentamicin sulfate	1305047-01	1
eurho	Gentamicin sulfate	1711025-01	1
EuRho	Gentamicin sulfate	1711025-01	2
EuRho	Gentamicin sulfate	1808013-01	4
EuRho	Gentamicin sulfate	190703601	1
EuRho	Gentamicin sulfate	1907036-01	2
EuRho	Gentamicin sulfate	2203032-01	1
EuRho	Gentamicin sulfate	FG1112482	1
Eurimpharm1	Gentamicin sulfate	1604054-01	1
euro AHD	Gentamicin sulfate	1711025-015586	1
Euro Gehe	Gentamicin sulfate	1907036-01	1
Euro Noweda	Gentamicin sulfate	FG1802035	1
Euro OTC	Gentamicin sulfate		1
Euro OTC	Gentamicin sulfate	1106016-01	3
Euro OTC	Gentamicin sulfate	1106016-02	3
Euro OTC	Gentamicin sulfate	1106016-03	5
Euro OTC	Gentamicin sulfate	1205021-01	12
Euro OTC	Gentamicin sulfate	1205021-02	17
Euro OTC	Gentamicin sulfate	1305047	1
Euro OTC	Gentamicin sulfate	130504701	1
Euro OTC	Gentamicin sulfate	1305047-01	9
Euro OTC	Gentamicin sulfate	130504703	2
Euro OTC	Gentamicin sulfate	1305047-03	12
Euro OTC	Gentamicin sulfate	13189607	1
Euro OTC	Gentamicin sulfate	1407024	1
Euro OTC	Gentamicin sulfate	1407024-01	6
Euro OTC	Gentamicin sulfate	1407024-02	1
Euro OTC	Gentamicin sulfate	140702403	1
Euro OTC	Gentamicin sulfate	1407024-03	2
Euro OTC	Gentamicin sulfate	140702404	3
Euro OTC	Gentamicin sulfate	1407024-04	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Gentamicin sulfate	150601601	1
Euro OTC	Gentamicin sulfate	1506016-01	18
Euro OTC	Gentamicin sulfate	150601602	2
Euro OTC	Gentamicin sulfate	1506016-02	29
Euro OTC	Gentamicin sulfate	15258816	2
Euro OTC	Gentamicin sulfate	160405-03	1
Euro OTC	Gentamicin sulfate	160405401	1
Euro OTC	Gentamicin sulfate	1604054-01	25
Euro OTC	Gentamicin sulfate	1604054-02	13
Euro OTC	Gentamicin sulfate	1604054-03	3
Euro OTC	Gentamicin sulfate	1604054-3	1
Euro OTC	Gentamicin sulfate	161003601	3
Euro OTC	Gentamicin sulfate	1610036-01	22
Euro OTC	Gentamicin sulfate	1610036-015339	1
Euro OTC	Gentamicin sulfate	161003602	1
Euro OTC	Gentamicin sulfate	1610036-02	17
Euro OTC	Gentamicin sulfate	171025-02	1
Euro OTC	Gentamicin sulfate	1711025-01	37
Euro OTC	Gentamicin sulfate	171102502	1
Euro OTC	Gentamicin sulfate	1711025-02	16
Euro OTC	Gentamicin sulfate	17358609	2
Euro OTC	Gentamicin sulfate	1801813-02	1
Euro OTC	Gentamicin sulfate	180208G/1711025-01	1
Euro OTC	Gentamicin sulfate	1808013-01	27
Euro OTC	Gentamicin sulfate	180801302	2
Euro OTC	Gentamicin sulfate	1808013-02	35
Euro OTC	Gentamicin sulfate	180813-02	1
Euro OTC	Gentamicin sulfate	18C12-B02-349519	1
Euro OTC	Gentamicin sulfate	18G06-B09	1
Euro OTC	Gentamicin sulfate	1907035-01	1
Euro OTC	Gentamicin sulfate	1907036	2
Euro OTC	Gentamicin sulfate	190703601	6
Euro OTC	Gentamicin sulfate	1907036-01	54
Euro OTC	Gentamicin sulfate	1907038-01	1
Euro OTC	Gentamicin sulfate	20003058-01	1
Euro OTC	Gentamicin sulfate	2003052-01	1
Euro OTC	Gentamicin sulfate	2003053-01	1
Euro OTC	Gentamicin sulfate	2003058	3
Euro OTC	Gentamicin sulfate	2003058-01	46
Euro OTC	Gentamicin sulfate	200305802	2
Euro OTC	Gentamicin sulfate	2003058-02	58
Euro OTC	Gentamicin sulfate	2003058-42	1
Euro OTC	Gentamicin sulfate	2107013-01	7
Euro OTC	Gentamicin sulfate	2107013-02	18
Euro OTC	Gentamicin sulfate	22000754003	1
Euro OTC	Gentamicin sulfate	2203032-01	6
Euro OTC	Gentamicin sulfate	2911034-02	1
Euro OTC	Gentamicin sulfate	4318A-01582	1
Euro OTC	Gentamicin sulfate	4988304	1
Euro OTC	Gentamicin sulfate	80616-2	1
Euro OTC	Gentamicin sulfate	FG11112482	1
Euro OTC	Gentamicin sulfate	FG1501009	1
Euro OTC	Gentamicin sulfate	FG1706157	1
Euro OTC	Gentamicin sulfate	FG1709241	2
Euro OTC	Gentamicin sulfate	FG1802035	1
Euro/Krieger	Gentamicin sulfate	1711025-02	1
Euro/Phönix	Gentamicin sulfate	1808013-01	1
Euro/Phönix	Gentamicin sulfate	1907036-01	1
Euro/Phönix	Gentamicin sulfate	2003058-0208	1
Euro/Sana	Gentamicin sulfate	1808013-01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
EuRoh/ Gehe	Gentamicin sulfate	17358616	1
EuRoh/ Gehe	Gentamicin sulfate	190703601	1
Euroo/Noweda	Gentamicin sulfate	2003058-02	1
Euroo/Phoenix	Gentamicin sulfate	1305047-03	1
Fagron	Gentamicin sulfate		1
Fagron	Gentamicin sulfate	10A29-N06	1
Fagron	Gentamicin sulfate	10C22N02	1
Fagron	Gentamicin sulfate	11/09-N10	1
Fagron	Gentamicin sulfate	1106016-01	1
Fagron	Gentamicin sulfate	11604054-01	1
Fagron	Gentamicin sulfate	11k21-n17	1
Fagron	Gentamicin sulfate	11K21-N17	2
Fagron	Gentamicin sulfate	1205021-02	1
Fagron	Gentamicin sulfate	1221-n02	1
Fagron	Gentamicin sulfate	12B21-N02	2
Fagron	Gentamicin sulfate	12D26-N05	9
Fagron	Gentamicin sulfate	12D6-N05	1
Fagron	Gentamicin sulfate	12G04-N16	2
Fagron	Gentamicin sulfate	12l17-no2	1
Fagron	Gentamicin sulfate	13/19-B05	1
Fagron	Gentamicin sulfate	13/19-B05-286568	1
Fagron	Gentamicin sulfate	13189607	1
Fagron	Gentamicin sulfate	1319-B05-286565	1
Fagron	Gentamicin sulfate	13D24-N05	8
Fagron	Gentamicin sulfate	13F13-N01	1
Fagron	Gentamicin sulfate	13I19-B05	1
Fagron	Gentamicin sulfate	13I19-B05-286568	1
Fagron	Gentamicin sulfate	14081307	2
Fagron	Gentamicin sulfate	14A30-B04	3
Fagron	Gentamicin sulfate	14a30-b04-290858	1
Fagron	Gentamicin sulfate	14A30-B04-290858	1
Fagron	Gentamicin sulfate	14A30-B04-290861	2
Fagron	Gentamicin sulfate	14E08-B03	2
Fagron	Gentamicin sulfate	14E08-B03-294835	2
Fagron	Gentamicin sulfate	14E08-B03-294841	1
Fagron	Gentamicin sulfate	14E08-B03-294848	5
Fagron	Gentamicin sulfate	14e08b03300619	1
Fagron	Gentamicin sulfate	14E08-B03-300619	1
Fagron	Gentamicin sulfate	14K28-B06	3
Fagron	Gentamicin sulfate	14K28-B06_303646	1
Fagron	Gentamicin sulfate	14K28-B06-301951	1
Fagron	Gentamicin sulfate	14k28-b06-303640	2
Fagron	Gentamicin sulfate	14k28-B06-303640	1
Fagron	Gentamicin sulfate	14K28-B06-303640	4
Fagron	Gentamicin sulfate	14K28B06303646	2
Fagron	Gentamicin sulfate	14K28-B06-303646	5
Fagron	Gentamicin sulfate	15121722	2
Fagron	Gentamicin sulfate	15258802	1
Fagron	Gentamicin sulfate	15258816	2
Fagron	Gentamicin sulfate	15803-B07-309482	1
Fagron	Gentamicin sulfate	15B03-B07	1
Fagron	Gentamicin sulfate	15b03-b07-309482	1
Fagron	Gentamicin sulfate	15B03-B07-309482	2
Fagron	Gentamicin sulfate	15E04-B05-316255	2
Fagron	Gentamicin sulfate	15E04-B05-319740	1
Fagron	Gentamicin sulfate	15G29-B09-320305	3
Fagron	Gentamicin sulfate	15G29-B09-322928	1
Fagron	Gentamicin sulfate	15G29B09322936	1
Fagron	Gentamicin sulfate	15G29-B09-322936	2
Fagron	Gentamicin sulfate	15G29-B09-322945	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Gentamicin sulfate	15G29B0932632	1
Fagron	Gentamicin sulfate	15G29-B09-326632	4
Fagron	Gentamicin sulfate	15G29-B09-326635	2
Fagron	Gentamicin sulfate	16829-B01-328731	1
Fagron	Gentamicin sulfate	16B29-B01	1
Fagron	Gentamicin sulfate	16B29-B01-328731	4
Fagron	Gentamicin sulfate	16-B-29-B01-328731	1
Fagron	Gentamicin sulfate	16b29-b01-328915	1
Fagron	Gentamicin sulfate	16B29-B01-328915	2
Fagron	Gentamicin sulfate	17099606	1
Fagron	Gentamicin sulfate	17099608	1
Fagron	Gentamicin sulfate	1711025-01	1
Fagron	Gentamicin sulfate	17G27-B05	1
Fagron	Gentamicin sulfate	17G27-B05-340121	2
Fagron	Gentamicin sulfate	17k16-B09-343323	1
Fagron	Gentamicin sulfate	17K16-B09-343323	1
Fagron	Gentamicin sulfate	17K-16-B09-343323	1
Fagron	Gentamicin sulfate	180810051	1
Fagron	Gentamicin sulfate	18C12-B02	3
Fagron	Gentamicin sulfate	18C12-B02-349025	7
Fagron	Gentamicin sulfate	18C12-B02-349026	2
Fagron	Gentamicin sulfate	18C12-B02-349519	1
Fagron	Gentamicin sulfate	18C12-B02-350	1
Fagron	Gentamicin sulfate	18C12B02350204	1
Fagron	Gentamicin sulfate	18C12-B02-350204	4
Fagron	Gentamicin sulfate	18G06-B09	2
Fagron	Gentamicin sulfate	18G06-B09-351916	6
Fagron	Gentamicin sulfate	18G06-B09-354797	9
Fagron	Gentamicin sulfate	1914Q-01582	1
Fagron	Gentamicin sulfate	19A22-B05-191434	18
Fagron	Gentamicin sulfate	19-B05-286568	1
Fagron	Gentamicin sulfate	19G17-805-193462	1
Fagron	Gentamicin sulfate	19G17-B05-193462	7
Fagron	Gentamicin sulfate	19G17-BO5-193462	2
Fagron	Gentamicin sulfate	19J15-B18-195524	2
Fagron	Gentamicin sulfate	2003058-02	1
Fagron	Gentamicin sulfate	20820-801-197708	1
Fagron	Gentamicin sulfate	20B20-B01	1
Fagron	Gentamicin sulfate	20B20-B01-1977008	1
Fagron	Gentamicin sulfate	20B20-B01-197708	12
Fagron	Gentamicin sulfate	20B20-B01-200399	1
Fagron	Gentamicin sulfate	20B20-B1-197708	1
Fagron	Gentamicin sulfate	20G27-802-202130	1
Fagron	Gentamicin sulfate	20G27-B02-201922	3
Fagron	Gentamicin sulfate	20G27-B02-202130	1
Fagron	Gentamicin sulfate	2107013-02	1
Fagron	Gentamicin sulfate	210920013	1
Fagron	Gentamicin sulfate	21D23-B07-213630	3
Fagron	Gentamicin sulfate	21D23-B07-215441	1
Fagron	Gentamicin sulfate	21I20-B09	1
Fagron	Gentamicin sulfate	21I20-B09-213601	2
Fagron	Gentamicin sulfate	22C17-B10-218675	2
Fagron	Gentamicin sulfate	22C17-B10-223074	1
Fagron	Gentamicin sulfate	22F28-B02-223061	2
Fagron	Gentamicin sulfate	5214A-01582	1
Fagron	Gentamicin sulfate	B01-1977008	2
Fagron	Gentamicin sulfate	B02-2019202	2
Fagron	Gentamicin sulfate	B02-3502004	2
Fagron	Gentamicin sulfate	B05-1934602	3
Fagron	Gentamicin sulfate	B09-3547907	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Gentamicin sulfate	FG1212646	1
Fagron	Gentamicin sulfate	FG1305122	1
Fagron	Gentamicin sulfate	FG1709255	1
Fagron	Gentamicin sulfate	FG1711309	2
Fargon	Gentamicin sulfate	13D24-N05	1
Fargon	Gentamicin sulfate	16b29-b01-328915	1
Fargon	Gentamicin sulfate	190110014	1
Fargron/AHD	Gentamicin sulfate	12G04-N16	1
Fuijan/Noweda	Gentamicin sulfate	18300108	1
Fuijan/Noweda	Gentamicin sulfate	192564009	1
Fuijan/Noweda	Gentamicin sulfate	FG1709243	3
Fujan	Gentamicin sulfate	2003058-02	1
Fujian FP / Gehe	Gentamicin sulfate	192564002	1
Fujian Fukang Pharm....	Gentamicin sulfate	17358603	1
Fujian Fukang Pharma...	Gentamicin sulfate	14A30-B04-290861	1
Fujian Fukang Pharma...	Gentamicin sulfate	14E08-B03-300619	1
Fujian Fukang Pharma...	Gentamicin sulfate	2003058-02	3
Fujian Fukang Pharma...	Gentamicin sulfate	12G04-N16	2
Fujian Fukang Pharma...	Gentamicin sulfate	14E08-B03-294848	1
Fujian/Noweda	Gentamicin sulfate	FG1802035	2
Fujian	Gentamicin sulfate	FG1706157	1
Gehe am 24.2.14	Gentamicin sulfate	1305047-01	1
Gehe amax	Gentamicin sulfate	1711025-01	1
Gehe amax	Gentamicin sulfate	2003058-01	1
Gehe/EuRho	Gentamicin sulfate	2203032-01	1
Gehe/Euro	Gentamicin sulfate	1610036-02	1
Gehe	Gentamicin sulfate		1
Gehe	Gentamicin sulfate	12146604	1
Gehe	Gentamicin sulfate	13205007	1
Gehe	Gentamicin sulfate	14353505	1
Gehe	Gentamicin sulfate	15226517	1
GEHE	Gentamicin sulfate	15258808	1
GEHE	Gentamicin sulfate	15258815	1
Gehe	Gentamicin sulfate	15258818	1
Gehe	Gentamicin sulfate	15E04-B05-319740	1
Gehe	Gentamicin sulfate	1610036-01	1
Gehe	Gentamicin sulfate	17099606	1
Gehe	Gentamicin sulfate	1711025-01	1
GEHE	Gentamicin sulfate	17358603	2
Gehe	Gentamicin sulfate	17358609	1
GEHE	Gentamicin sulfate	17358609	1
Gehe	Gentamicin sulfate	1808013-01	1
Gehe	Gentamicin sulfate	1808013-02	1
Gehe	Gentamicin sulfate	18300103	1
Gehe	Gentamicin sulfate	18300108	1
Gehe	Gentamicin sulfate	18300109	2
GEHE	Gentamicin sulfate	18300109	1
Gehe	Gentamicin sulfate	1907036-01	1
Gehe	Gentamicin sulfate	19A22-B05-191434	1
Gehe	Gentamicin sulfate	19G17-B05-193462	1
Gehe	Gentamicin sulfate	20004482004	1
Gehe	Gentamicin sulfate	2002058-01	1
Gehe	Gentamicin sulfate	22000754013	2
Gehe	Gentamicin sulfate	22C17-B10-223074	1
Gehe	Gentamicin sulfate	FG1307194	1
Geilenkirchen	Gentamicin sulfate	15258816	1
Geilenkirchen	Gentamicin sulfate	18300104	1
Hedinger	Gentamicin sulfate	1711025-01	1
Ichthyol/ALH	Gentamicin sulfate	15258810	1
Jenne	Gentamicin sulfate	20004482002	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Jenne	Gentamicin sulfate	20004483014	1
Jenne	Gentamicin sulfate	22000754013	1
Jenne	Gentamicin sulfate	23001024004	1
Kehr	Gentamicin sulfate	110036-02	1
Kehr	Gentamicin sulfate	22000754003	1
Klosterring	Gentamicin sulfate	15G29-B09	1
Mömerzheim	Gentamicin sulfate	1711025-01	1
Nachprüfung	Gentamicin sulfate	123456	1
Noweda Taucha	Gentamicin sulfate	20004483014	1
Noweda Taucha	Gentamicin sulfate	2003058-02	1
Noweda/ Caesar&Loren…	Gentamicin sulfate	192564002	1
Noweda	Gentamicin sulfate	12146602	1
Noweda	Gentamicin sulfate	1305005	1
Noweda	Gentamicin sulfate	13189607	1
Noweda	Gentamicin sulfate	13189611	1
Noweda	Gentamicin sulfate	13189612	1
Noweda	Gentamicin sulfate	140702404	1
Noweda	Gentamicin sulfate	14353504	1
Noweda	Gentamicin sulfate	15226514	1
Noweda	Gentamicin sulfate	15258818	1
Noweda	Gentamicin sulfate	1711025-02	1
Noweda	Gentamicin sulfate	17358616	2
Noweda	Gentamicin sulfate	17358623	1
Noweda	Gentamicin sulfate	18300108	2
Noweda	Gentamicin sulfate	1907036-01	2
noweda	Gentamicin sulfate	192564003	1
Noweda	Gentamicin sulfate	192564003	1
Noweda	Gentamicin sulfate	20004483013	1
Noweda	Gentamicin sulfate	210920013	1
Noweda	Gentamicin sulfate	22000754003	1
Noweda	Gentamicin sulfate	22000754006	1
Noweda	Gentamicin sulfate	23001024004	1
ph euro	Gentamicin sulfate	2003058-01	1
PHOENIX 10.03.2014	Gentamicin sulfate	1305047	1
Phoenix	Gentamicin sulfate	12D26-N05	1
Phoenix	Gentamicin sulfate	1305047-03	1
Phoenix	Gentamicin sulfate	15226501	1
Phoenix	Gentamicin sulfate	15226502	1
Phoenix	Gentamicin sulfate	15258816	1
Phoenix	Gentamicin sulfate	1604054-02	1
Phoenix	Gentamicin sulfate	16b29-b01-328731	1
Phoenix	Gentamicin sulfate	17099603	1
Phoenix	Gentamicin sulfate	1711025-02	2
phoenix	Gentamicin sulfate	17358603	1
Phoenix	Gentamicin sulfate	17358603	1
Phoenix	Gentamicin sulfate	17G27-B05-340121	1
Phoenix	Gentamicin sulfate	18300108	1
Phoenix	Gentamicin sulfate	18300113	1
Phoenix	Gentamicin sulfate	20004483001	1
Phoenix	Gentamicin sulfate	2003058-01	1
Phoenix	Gentamicin sulfate	22000754003	1
Phoenix	Gentamicin sulfate	23001024005	1
Phoenix	Gentamicin sulfate	3404	1
Phönix Gotha	Gentamicin sulfate	13189611	1
Phönix	Gentamicin sulfate	11113309	1
phönix	Gentamicin sulfate	1214605	1
Phönix	Gentamicin sulfate	12146602	1
Phönix	Gentamicin sulfate	13189611	1
Phönix	Gentamicin sulfate	14353502	1
PHÖNIX	Gentamicin sulfate	15226514	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Gentamicin sulfate	15258818	1
Phönix	Gentamicin sulfate	17099603	1
Phönix	Gentamicin sulfate	17099604	1
phönix	Gentamicin sulfate	18300103	1
Phönix	Gentamicin sulfate	18300109	2
Phönix	Gentamicin sulfate	192564009	1
PHÖNIX	Gentamicin sulfate	20004483001	1
Phönix	Gentamicin sulfate	2003058-01	2
phönix	Gentamicin sulfate	22000754006	1
Phönix	Gentamicin sulfate	22000754013	1
Phönix	Gentamicin sulfate	23001024004	2
Phönix	Gentamicin sulfate	3141	1
Sanacorp 06.01.15 EK 6,20	Gentamicin sulfate	1305047-03	1
Sanacorp WE: 28.09.1…	Gentamicin sulfate	15258825	1
Sanacorp	Gentamicin sulfate	1305047-03	1
Sanacorp	Gentamicin sulfate	13189607	1
Sanacorp	Gentamicin sulfate	13189608	1
Sanacorp	Gentamicin sulfate	161003601	1
Sanacorp	Gentamicin sulfate	1610036-01	2
Sanacorp	Gentamicin sulfate	1610036-02	1
Sanacorp	Gentamicin sulfate	161036-02	1
Sanacorp	Gentamicin sulfate	1711025-02	1
Sanacorp	Gentamicin sulfate	17358603	1
Sanacorp	Gentamicin sulfate	17358604	1
Sanacorp	Gentamicin sulfate	17358618	1
Sanacorp	Gentamicin sulfate	18300109	1
Sanacorp	Gentamicin sulfate	18300112	1
sanacorp	Gentamicin sulfate	18300113	1
Sanacorp	Gentamicin sulfate	18300113	1
Sanacorp	Gentamicin sulfate	18C12-B02-349026	1
Sanacorp	Gentamicin sulfate	19G17-B05-193462	1
Sanacorp	Gentamicin sulfate	2003058-02	1
Sanacorp	Gentamicin sulfate	2203032-01	1
Sanacorp	Gentamicin sulfate	23001024004	1
Sanacorp	Gentamicin sulfate	23001024005	1
Sanacorp	Gentamicin sulfate	FG1711309	1
vdl	Gentamicin sulfate	12146602	1
Yantai Justaware Ph.…	Gentamicin sulfate	14081307	1
Yantai Justaware Ph.…	Gentamicin sulfate	14K28-B06_303646	1
Yantai Justaware Pha…	Gentamicin sulfate	14K28-B06	1

- 233 530 spectra from 1515 *Apo-Ident* customers from a total of 48 881 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Gentamicin sulfate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gentamicin sulfate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	1015	0	151 947
Type B	0	948	2	201 134
Type C	0	2447	90	233 530

The substance/substance group *Gentamicin sulfate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.4089 %)
Type B	100.0000 % (> 99.9912 %)	99.7895 % (> 99.4737 %)
Type C	100.0000 % (> 99.9007 %)	96.4525 % (> 96.3343 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20661	20661	0.00	115.09
21081	21837	4.26	118.02
21578	25201	43.04	84.88
21580	21837	7.14	115.85
21582	21582	0.00	113.69
21684	21582	5.22	113.06
21697	21697	0.00	111.94
21837	21837	0.00	114.16
22604	21837	3.65	117.53
22857	22857	0.00	126.51
23210	21837	6.91	115.20
23782	23782	0.00	116.07
23882	23882	0.00	114.56
24866	24866	0.00	114.11
25180	22857	21.51	122.85
25201	25201	0.00	99.34
25252	25252	0.00	118.07
25638	25638	0.00	96.47

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Glucose**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20982-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Glucose; Glucosum

Special notes

When selecting the *Glucose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Glucose	6	2	250

Second-stage model

For differentiation of the substance/substance group *Glucose* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Glucose* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	84.70	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Glucose* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Glucose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Glucose	12294514	20982	40	1402475
Caelo	Glucose	14033901	21363	40	20140214
Caelo	Glucose	14142310	21703	45	20140523
Caelo	Glucose	16050501	22586	40	20160317
Caelo	Glucose	190380	24511	40	20190411*
Caelo	Glucose	22002306	26366	40	20220909*
Caelo	Glucose	22002306	26366SI	20	20220909*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 265 spectra of 7 reference samples from the substance/substance group *Glucose*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 697 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Glucose*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Glucose	16157401	23583	40
Caelo	Glucose	180129	23820	40

- 202 004 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1521 spectra from 309 *Apo-Ident* customers from 257 batches from the substance/substance group *Glucose*.

- Among them are spectra of independent samples from 249 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Glucose		1
	Glucose	21002549009	1
	Glucose	21002549010	1
	Glucose	21002549012	7
	Glucose	21002549014	1
	Glucose	22002306002	1
	Glucose	22002306003	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
	Glucose	22002306006	10
	Glucose	22002306008	1
	Glucose	22002306010	2
	Glucose	22003206006	1
21.03.2017	Glucose	6910499	1
AHD	Glucose	14033908	1
AHD	Glucose	21002549004	1
AHD	Glucose	21002549014	1
AHD	Glucose	22002306010	1
Aliance Healthcare	Glucose	21002549012	2
Allianc. Healthc. /c	Glucose	16050510	1
Anzag	Glucose	13329505	1
Apotheke/Defektur Mi...	Glucose		1
Apotheke-SiO2-Mischung	Glucose	18/15	1
Audor Pharma	Glucose	16157402	3
Bombastus	Glucose	160505202	1
Caelo	Glucose	1001313393	1
Caelo	Glucose	10091503	1
Caelo	Glucose	1061703	1
Caelo	Glucose	106213393	1
Caelo	Glucose	1114A03393	1
Caelo	Glucose	11358823	1
Caelo	Glucose	12041801	1
Caelo	Glucose	120718A	1
Caelo	Glucose	12141705	1
Caelo	Glucose	12141706	3
Caelo	Glucose	12141714	2
Caelo	Glucose	12141715	1
Caelo	Glucose	12141717	1
Caelo	Glucose	12141718	3
Caelo	Glucose	12294505	3
Caelo	Glucose	12294509	2
Caelo	Glucose	12294509-3425311150	1
Caelo	Glucose	12294510	3
Caelo	Glucose	12294511	1
Caelo	Glucose	12294514	2
Caelo	Glucose	12294515	2
Caelo	Glucose	12294517	1
Caelo	Glucose	12294519	1
Caelo	Glucose	13041501	1
Caelo	Glucose	1317815	1
Caelo	Glucose	13178701	2
Caelo	Glucose	13178702	1
Caelo	Glucose	13178704	3
Caelo	Glucose	13178707	2
Caelo	Glucose	13178711	2
Caelo	Glucose	13178712	1
Caelo	Glucose	13178715	4
Caelo	Glucose	13178716	1
Caelo	Glucose	13178718	1
Caelo	Glucose	13329501	3
Caelo	Glucose	13329503	3
Caelo	Glucose	13329504	2
Caelo	Glucose	13329507	1
Caelo	Glucose	13329512	7
Caelo	Glucose	14033901	2
Caelo	Glucose	14033902	4
Caelo	Glucose	14033906	5
Caelo	Glucose	14033907	5
Caelo	Glucose	14033908	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glucose	14051401	1
Caelo	Glucose	14051802	1
Caelo	Glucose	14142301	1
Caelo	Glucose	14142303	3
Caelo	Glucose	14142304	1
Caelo	Glucose	14142308	1
Caelo	Glucose	14142310	5
Caelo	Glucose	14142313	2
Caelo	Glucose	14142314	3
Caelo	Glucose	1415U-03393	1
Caelo	Glucose	14319302	1
Caelo	Glucose	14319304	6
Caelo	Glucose	14319308	1
Caelo	Glucose	14319309	3
Caelo	Glucose	14319310	2
Caelo	Glucose	1439304	1
Caelo	Glucose	15021801	1
Caelo	Glucose	15051301	1
Caelo	Glucose	15081831	1
Caelo	Glucose	1509500	3
Caelo	Glucose	15095001	8
Caelo	Glucose	15095003	4
Caelo	Glucose	15095004	3
Caelo	Glucose	15095005	2
Caelo	Glucose	15148801	4
Caelo	Glucose	15148802	6
Caelo	Glucose	15148803	1
Caelo	Glucose	15148807	4
Caelo	Glucose	15148808	4
Caelo	Glucose	15148809	1
Caelo	Glucose	15148810	4
Caelo	Glucose	15148813	1
Caelo	Glucose	15329001	6
Caelo	Glucose	15329002	2
Caelo	Glucose	15329004	4
Caelo	Glucose	15329005	4
Caelo	Glucose	15329006	11
Caelo	Glucose	15329008	2
Caelo	Glucose	15329010	2
Caelo	Glucose	160308G	1
Caelo	Glucose	16050501	19
Caelo	Glucose	16050502	12
Caelo	Glucose	16050503	23
Caelo	Glucose	16050504	1
Caelo	Glucose	16050507	3
Caelo	Glucose	16050508	3
Caelo	Glucose	16050510	3
Caelo	Glucose	16101204	1
Caelo	Glucose	16101205	1
Caelo	Glucose	1614U3393	1
Caelo	Glucose	16157402	5
Caelo	Glucose	16157403	28
Caelo	Glucose	16157403160117/1	1
Caelo	Glucose	16157406	24
Caelo	Glucose	16157406160117/2	1
Caelo	Glucose	16157411	10
Caelo	Glucose	16328801	16
Caelo	Glucose	16328803	14
Caelo	Glucose	16328805	21
Caelo	Glucose	16328807	6

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glucose	16328811	9
Caelo	Glucose	16328812	16
Caelo	Glucose	16328813	1
Caelo	Glucose	1638803	1
Caelo	Glucose	1650502	1
Caelo	Glucose	17041701	1
Caelo	Glucose	17111803	1
Caelo	Glucose	18012902	31
Caelo	Glucose	1801290246/18	1
Caelo	Glucose	18012903	3
Caelo	Glucose	18012905	13
Caelo	Glucose	18012907	39
Caelo	Glucose	18012909	14
Caelo	Glucose	18012910	2
Caelo	Glucose	18012911	6
Caelo	Glucose	18012912	29
Caelo	Glucose	18012913	8
Caelo	Glucose	18012914	17
Caelo	Glucose	18012915	26
Caelo	Glucose	18012916	1
Caelo	Glucose	18012917	10
Caelo	Glucose	18012920	4
Caelo	Glucose	18012921	36
Caelo	Glucose	18012922	7
Caelo	Glucose	18012923	3
Caelo	Glucose	18012926	3
Caelo	Glucose	18111702	1
Caelo	Glucose	1812913	1
Caelo	Glucose	19028005	1
Caelo	Glucose	190320011	1
Caelo	Glucose	190380002	5
Caelo	Glucose	190380003	40
Caelo	Glucose	190380006	8
Caelo	Glucose	190380007	1
Caelo	Glucose	190380009	32
Caelo	Glucose	19038001	7
Caelo	Glucose	190380011	2
Caelo	Glucose	19038002	42
Caelo	Glucose	19038003	6
Caelo	Glucose	19038005	12
Caelo	Glucose	19038006	14
Caelo	Glucose	19038007	42
Caelo	Glucose	19080009	2
Caelo	Glucose	1914I03393	1
Caelo	Glucose	20001066020	2
Caelo	Glucose	20004066	1
Caelo	Glucose	20004066001	5
Caelo	Glucose	20004066002	3
Caelo	Glucose	20004066004	31
Caelo	Glucose	200040660042x	1
Caelo	Glucose	20004066005	4
Caelo	Glucose	200040660058	1
Caelo	Glucose	20004066006	6
Caelo	Glucose	20004066008	49
Caelo	Glucose	20004066010	8
Caelo	Glucose	20004066011	5
Caelo	Glucose	20004066013	1
Caelo	Glucose	20004066014	1
Caelo	Glucose	20004066015	6
Caelo	Glucose	20004066017	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glucose	20004066018	19
Caelo	Glucose	20004066019	1
Caelo	Glucose	20004066020	4
Caelo	Glucose	20004066021	6
Caelo	Glucose	20004066023	12
Caelo	Glucose	2000406608	1
Caelo	Glucose	2000406611	1
Caelo	Glucose	2004066008	1
Caelo	Glucose	2004066014	1
Caelo	Glucose	2004066021	1
Caelo	Glucose	2004066023	1
Caelo	Glucose	200406604	1
Caelo	Glucose	2013Q-03393	1
Caelo	Glucose	2021902	1
Caelo	Glucose	2051701	1
Caelo	Glucose	208223393	1
Caelo	Glucose	210002549007	1
Caelo	Glucose	210002549012	1
Caelo	Glucose	2100254009	1
Caelo	Glucose	21002549	1
Caelo	Glucose	21002549002	2
Caelo	Glucose	21002549003	29
Caelo	Glucose	21002549004	8
Caelo	Glucose	21002549007	23
Caelo	Glucose	21002549008	2
Caelo	Glucose	21002549009	6
Caelo	Glucose	21002549012	17
Caelo	Glucose	21002549013	3
Caelo	Glucose	21002549014	1
Caelo	Glucose	2102201301	1
Caelo	Glucose	214U-03393	1
Caelo	Glucose	220002306003	1
Caelo	Glucose	23091401	1
Caelo	Glucose	250004066021	1
Caelo	Glucose	25061204	1
Caelo	Glucose	2513M03393	1
Caelo	Glucose	26041303	1
Caelo	Glucose	28111714	1
Caelo	Glucose	2x18012915	1
Caelo	Glucose	3121402	1
Caelo	Glucose	3214M-03393	1
Caelo	Glucose	3513I-03393	1
Caelo	Glucose	3918M-03393	1
Caelo	Glucose	402313393	2
Caelo	Glucose	4071505	1
Caelo	Glucose	4117I-03393	1
Caelo	Glucose	4313Q3393	1
Caelo	Glucose	4616I-03393	1
Caelo	Glucose	4713l-03393	1
Caelo	Glucose	5013I3393	1
Caelo	Glucose	5081401	1
Caelo	Glucose	551616157406	1
Caelo	Glucose	6031505	1
Caelo	Glucose	6071717	1
Caelo	Glucose	69010513	1
Caelo	Glucose	7091705	1
Caelo	Glucose	712213393	1
Caelo	Glucose	8031703	1
Caelo	Glucose	8091810	1
Caelo	Glucose	85(06910499)	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glucose	AKD14	1
Caelo	Glucose	I-180716-1605010	1
Caesar & Loretz GmbH...	Glucose	20004066018	2
Caesar & Loretz GmbH...	Glucose	20004066008	2
Caesar & Loretz GmbH...	Glucose	21002549005	1
Caesar & Loretz GmbH...	Glucose	20004066023	2
Caesar & Loretz GmbH...	Glucose	21002549009	1
Caesar & Loretz GmbH...	Glucose	18012921	3
Caesar & Loretz GmbH...	Glucose	20004066006	3
Caesar & Loretz GmbH/Gehe	Glucose	190380003	3
Caesar & Loretz GmbH/Gehe	Glucose	20004066011	1
Caesar & Loretz GmbH/Gehe	Glucose	21002549003	4
Caesar & Loretz GmbH/Gehe	Glucose	21002549007	1
Caesar & Loretz GmbH...	Glucose	19038002	2
Caesar & Loretz GmbH...	Glucose	21002549003	1
Caesar & Loretz GmbH...	Glucose	190380009	1
Caesar & Loretz GmbH...	Glucose	20004066013	1
Caesar & Loretz GmbH...	Glucose	20004066017	1
Caesar & Loretz GmbH...	Glucose	19038002	1
Caesar & Loretz GmbH...	Glucose	21002549003	1
Caesar & Loretz GmbH	Glucose	16157403	1
Caesar & Loretz GmbH	Glucose	18012909	1
Caesar & Loretz GmbH	Glucose	18012912	1
Caesar & Loretz GmbH	Glucose	18012915	2
Caesar & Loretz GmbH	Glucose	18012921	7
Caesar & Loretz GmbH	Glucose	18012922	2
Caesar & Loretz GmbH	Glucose	18012926	1
Caesar & Loretz GmbH	Glucose	190380002	4
Caesar & Loretz GmbH	Glucose	190380003	7
Caesar & Loretz GmbH	Glucose	190380005	1
Caesar & Loretz GmbH	Glucose	190380009	5
Caesar & Loretz GmbH	Glucose	19038001	3
Caesar & Loretz GmbH	Glucose	190380010	2
Caesar & Loretz GmbH	Glucose	19038002	1
Caesar & Loretz GmbH	Glucose	19038005	2
Caesar & Loretz GmbH	Glucose	19038006	1
Caesar & Loretz GmbH	Glucose	19038007	5
Caesar & Loretz GmbH	Glucose	20004066002	3
Caesar & Loretz GmbH	Glucose	20004066004	2
Caesar & Loretz GmbH	Glucose	20004066005	2
Caesar & Loretz GmbH	Glucose	20004066007	1
Caesar & Loretz GmbH	Glucose	20004066008	2
Caesar & Loretz GmbH	Glucose	20004066010	1
Caesar & Loretz GmbH	Glucose	20004066011	1
Caesar & Loretz GmbH	Glucose	20004066017	1
Caesar & Loretz GmbH	Glucose	20004066018	1
Caesar & Loretz GmbH	Glucose	20004066020	2
Caesar & Loretz GmbH	Glucose	20004066022	1
Caesar & Loretz GmbH	Glucose	21002549002	3
Caesar & Loretz GmbH	Glucose	21002549003	3
Caesar & Loretz GmbH	Glucose	21002549004	1
Caesar & Loretz GmbH	Glucose	21002549007	3
Caesar & Loretz GmbH	Glucose	21002549008	2
Caesar & Loretz GmbH	Glucose	21002549009	1
Caesar & Loretz GmbH	Glucose	21002549012	2
Caesar & Loretz GmbH	Glucose	21002549013	1
Caesar & Loretz GmbH	Glucose	21002549014	1
Caesar & Loretz GmbH	Glucose	210025949007	1
Caesar & Loretz Hild...	Glucose	18012921	1
Caesar & Loretz Hild...	Glucose	190380003	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz Hild...	Glucose	190380003190380009	1
Caesar & Loretz Hild...	Glucose	19038007	1
Caesar & Loretz Hilden	Glucose	18012914	2
Caesar & Loretz Hilden	Glucose	18012915	1
Caesar & Loretz Hilden	Glucose	19038002	3
Caesar & Loretz Hilden	Glucose	20004066004	1
Caesar & Loretz/ Pho...	Glucose	20004066004	2
Caesar & Loretz	Glucose	16157402	1
Caesar & Loretz	Glucose	18012923	1
Caesar u. Loretz GmbH	Glucose	190380003	2
Caesar u. Loretz GmbH	Glucose	190380009	1
Caesar u. Loretz GmbH	Glucose	20004066008	2
Caesar&Loretz GmbH	Glucose	19038006	3
Caesar&loretz,Anzag	Glucose	12294509	1
Caesar&Loretz	Glucose	15148808	1
Euro OTC	Glucose		1
Euro OTC	Glucose	15148808	1
Euro OTC	Glucose	16050501	1
Euro OTC	Glucose	16050502	2
Euro OTC	Glucose	18012905	3
Euro OTC	Glucose	18012922	1
Fagron	Glucose	13178716	1
Fagron	Glucose	14142303	1
Fagron	Glucose	15329005	2
Fiebig 02.05.2019	Glucose	18012915	1
Fiebig	Glucose	18012907	1
GEHE 17.07.2014	Glucose	14033907	1
Gehe 27.11.14	Glucose	14142309	1
Gehe Kassel	Glucose	14142313	1
GEHE	Glucose	13178715	1
Gehe	Glucose	16157403	2
GEHE	Glucose	16157406	1
GEHE	Glucose	16328801	1
Gehe	Glucose	16328803	1
Gehe	Glucose	16328805	2
GEHE	Glucose	16328805	1
Gehe	Glucose	163288205	1
Gehe	Glucose	18012902	1
GEHE	Glucose	18012902	2
Gehe	Glucose	18012907	2
GEHE	Glucose	18012907	4
Gehe	Glucose	18012912	1
GEHE	Glucose	18012912	2
Gehe	Glucose	18012914	1
Gehe	Glucose	18012915	2
GEHE	Glucose	18012915	4
Gehe	Glucose	18012921	2
Gehe	Glucose	190380003	7
Gehe	Glucose	19038002	3
GEHE	Glucose	19038002	2
Gehe	Glucose	19038003	1
Gehe	Glucose	19038007	1
Gehe	Glucose	20004066004	2
gehe	Glucose	22002306003	1
Geibo/Noweda	Glucose	18012907	1
Geibo	Glucose	190380003	1
Geibo	Glucose	19038007	2
Geilenkirchen	Glucose	18012902	1
Geilenkirchen	Glucose	18012921	3
Geilenkirchen	Glucose	190380009	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Geilenkirchen	Glucose	20004066023	1
Ichtyol-Ges HH/Sanacorp	Glucose	18012909	1
Jenne	Glucose	12141705	1
Klenk	Glucose	16050502	1
Max Jenne	Glucose	23002088001	1
Nachprüfung	Glucose		2
Noweda	Glucose	18012922	1
Noweda	Glucose	20004066004	1
Noweda	Glucose	20004066014	1
Noweda	Glucose	21002549007	4
Noweda	Glucose	21002549008	1
PHOENIX 30.05.2014	Glucose	13329514	1
PHOENIX 30.05.2014	Glucose	14033902	1
Phoenix	Glucose	14142310	1
Phoenix	Glucose	15148801	1
Phoenix	Glucose	15329010	2
Phoenix	Glucose	16050501	1
Phoenix	Glucose	16050503	4
Phoenix	Glucose	190380009	1
Phoenix	Glucose	191250611	1
Phönix/Fagon	Glucose	16328807	1
Phönix	Glucose	13178701	1
PHÖNIX	Glucose	16328805	2
PHÖNIX	Glucose	16328812	3
PHÖNIX	Glucose	18012902	1
Rondell Apotheke	Glucose	15329003	1
Sanacorp	Glucose	12294509	1
Sanacorp	Glucose	16328805	1
Sanacorp	Glucose	18012907	2
Sanacorp	Glucose	18012909	1
Sanacorp	Glucose	190380009	2
Sanacorp	Glucose	20004066023	1
Sanacorp	Glucose	2004066023	1
Sanacorp	Glucose	21002549008	1
sanacorp	Glucose	22002306003	1
Sanacorp	Glucose	22002306003	1
Sanacorp	Glucose	22002306006	4
Sanacorp	Glucose	23002088001	1
Sonnen-Apotheke Wefe…	Glucose	17/16	1
Sonnen-Apotheke Wefe…	Glucose	21/17Glucose-SiO2-M	1
Sonnen-Apotheke Wefe…	Glucose	34/16	1

- 234 546 spectra from 1515 *Apo-Ident* customers from a total of 49 003 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Glucose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Glucose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	265	0	152 697
Type B	0	80	0	202 004
Type C	0	1518	3	234 546

The substance/substance group *Glucose* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7358 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9007 %)	99.8028 % (> 99.6055 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20982	20982	0.00	218.11
21363	26366	10.79	227.54
21703	20982	6.16	222.64
22586	20982	4.10	222.40
24511	24511	0.00	238.58
26366	26366	0.00	244.18

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Glucose monohydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20031-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Glucose monohydrate; Glucosum monohydricum

Special notes

When selecting the *Glucose monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Glucose monohydrate	12	23	565

Second-stage model

For differentiation of the substance/substance group *Glucose monohydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Glucose monohydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	78.17	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Glucose monohydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Glucose monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Glucose monohydrate	171368	23304	40	20170601*
Caelo	Glucose monohydrate	173050	23802	40	20171110*
Caelo	Glucose monohydrate	20003964	25627	40	20210115*
Caelo	Glucose monohydrate	20003963	25637	40	20210115*
Caelo	Glucose monohydrate	20002144	25653	40	20200813*
Euro OTC	Glucose monohydrate	1509006	21905	60	20150914*
Euro OTC	Glucose monohydrate	1601016	22308	60	20160129*
Euro OTC	Glucose monohydrate	1604006	22538	40	20160511*
Euro OTC	Glucose monohydrate	1701002	23006	40	20170213*
Euro OTC	Glucose monohydrate	1807005	24162	40	20180718*
Fagron	Glucose monohydrate	11L19-N13	20799	40	20120105
Fagron	Glucose monohydrate	14B04-B01	21274	40	20140304

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 520 spectra of 12 reference samples from the substance/substance group *Glucose monohydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 12 different batches.

- 152 442 spectra from a total of 2830 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 970 spectra of 26 reference samples from the substance/substance group *Glucose monohydrate*.

- Among them are spectra of independent samples from 23 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Glucose monohydrate	16184807	23025	40
Caelo	Glucose monohydrate	190733	24506	40
Caelo	Glucose monohydrate	182174	24906	40
Caelo	Glucose monohydrate	22001899	26364	30
Caelo	Glucose monohydrate	24002353	27438	40
Euro OTC	Glucose monohydrate	1210034-02	21285	40
Euro OTC	Glucose monohydrate	1607024	22692	40
Euro OTC	Glucose monohydrate	1707004	23545	40
Euro OTC	Glucose monohydrate	1801009	23897	40
Euro OTC	Glucose monohydrate	1811020	24418	40
Euro OTC	Glucose monohydrate	1904029	24640	40
Euro OTC	Glucose monohydrate	1908012	24860	40
Euro OTC	Glucose monohydrate	2001006	25083	40
Euro OTC	Glucose monohydrate	2006007	25310	40
Euro OTC	Glucose monohydrate	2009024	25461	40
Euro OTC	Glucose monohydrate	2103027	25671	40
Euro OTC	Glucose monohydrate	2107024	25772	50
Euro OTC	Glucose monohydrate	2109008	25824	50
Euro OTC	Glucose monohydrate	2202015	26040	40
Euro OTC	Glucose monohydrate	2206018	26209	40
Euro OTC	Glucose monohydrate	2210005	26418	30
Euro OTC	Glucose monohydrate	2302007	26591	40
Euro OTC	Glucose monohydrate	2310008	26997	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Glucose monohydrate	22001899	26364SI	20
Euro OTC	Glucose monohydrate	2202015	26040SI	10
Euro OTC	Glucose monohydrate	2206018	26209SI	20

- 201 114 spectra from a total of 4022 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4533 spectra from 906 *Apo-Ident* customers from 575 batches from the substance/substance group *Glucose monohydrate*.

- Among them are spectra of independent samples from 565 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Glucose monohydrate		2
	Glucose monohydrate	21001886009	1
	Glucose monohydrate	2109008-01	1
	Glucose monohydrate	2109008-02	1
	Glucose monohydrate	22000756006	3
	Glucose monohydrate	22000756007	1
	Glucose monohydrate	22000756015	1
	Glucose monohydrate	22000756019	8
	Glucose monohydrate	22000756021	1
	Glucose monohydrate	22001899002	12
	Glucose monohydrate	22001899003	2
	Glucose monohydrate	22001899005	5
	Glucose monohydrate	22001899010	2
	Glucose monohydrate	22001899011	13
	Glucose monohydrate	2200756015	1
	Glucose monohydrate	2202015-03	1
	Glucose monohydrate	22021899011	1
	Glucose monohydrate	2206018-01	3
	Glucose monohydrate	2206018-02	1
	Glucose monohydrate	2210005-01	3
	Glucose monohydrate	221000502	1
	Glucose monohydrate	2210005-02	6
	Glucose monohydrate	23000211001	2
	Glucose monohydrate	23000211002	1
	Glucose monohydrate	23000211004	1
	Glucose monohydrate	23000211005	9
	Glucose monohydrate	23000211006	2
	Glucose monohydrate	23000211010	2
	Glucose monohydrate	230008-01	1
	Glucose monohydrate	23003430002	1
	Glucose monohydrate	2302007-01	10
	Glucose monohydrate	2302007-02	4
	Glucose monohydrate	23100008-02	1
	Glucose monohydrate	2310008-01	6
	Glucose monohydrate	24000422002	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Glucose monohydrate	24000422004	1
	Glucose monohydrate	24000422005	1
	Glucose monohydrate	557473	1
73098/Gehe	Glucose monohydrate	E388S	1
ACM	Glucose monohydrate	KNC1164J15	1
ACM	Glucose monohydrate	KNC1282J14	1
AHD	Glucose monohydrate	14102407	1
AHD	Glucose monohydrate	21001886013	1
AHD	Glucose monohydrate	2202015-02	1
AHD	Glucose monohydrate	2210005-01	2
AHD	Glucose monohydrate	2310008-01	2
AHD	Glucose monohydrate	24000422004	1
Alliance/EurRho	Glucose monohydrate	2103027-01	1
Alliance	Glucose monohydrate	16049101	1
Alliance	Glucose monohydrate	22000756011	1
Alliance	Glucose monohydrate	22001899005	1
Alliance	Glucose monohydrate	2202015-02	1
Allianz Healthcare	Glucose monohydrate	19073305	1
allianz	Glucose monohydrate	1543409	1
Anzag	Glucose monohydrate	14334810	1
Anzag	Glucose monohydrate	16184808	1
Anzag	Glucose monohydrate	17005804	1
Anzag	Glucose monohydrate	17136805	1
api-ident / AHD	Glucose monohydrate	2009024-01	1
apo ident/Noweda	Glucose monohydrate	2103027-01	1
apo ident	Glucose monohydrate	202015-02	1
Apoident/ Phoenix	Glucose monohydrate	2009024-01	1
Apo-Ident/Phoenix	Glucose monohydrate	1701002-01	1
Apo-Ident/Phoenix	Glucose monohydrate	1707004-01	3
apo-ident	Glucose monohydrate	1604006-02	1
ApoIdent	Glucose monohydrate	2107024-02	1
ApoIdent	Glucose monohydrate	2206018-01	1
Apotheke im Forum	Glucose monohydrate	17010002-01	1
Audor Pharma	Glucose monohydrate	2202015-03	1
Audor Pharma	Glucose monohydrate	2206018-01	2
Audor Pharma	Glucose monohydrate	E732N	1
Beiersdorf/Phönix	Glucose monohydrate	L6209	1
Bombastus	Glucose monohydrate	14334802	2
Bombastus	Glucose monohydrate	15413410	1
Bombastus	Glucose monohydrate	16184810	2
Bombastus	Glucose monohydrate	1807005-01	1
Bombastus	Glucose monohydrate	18101901	2
Bombastus	Glucose monohydrate	18214703	3
Caello/Phönix	Glucose monohydrate	15095601	3
Caelo	Glucose monohydrate		3
Caelo	Glucose monohydrate	10159501	1
Caelo	Glucose monohydrate	1073303	1
Caelo	Glucose monohydrate	11021509	1
Caelo	Glucose monohydrate	11082014	1
Caelo	Glucose monohydrate	11082020	1
Caelo	Glucose monohydrate	111111111	1
Caelo	Glucose monohydrate	11314516	3
Caelo	Glucose monohydrate	11314519	1
Caelo	Glucose monohydrate	11314526	1
Caelo	Glucose monohydrate	11314528	8
Caelo	Glucose monohydrate	1134506	1
Caelo	Glucose monohydrate	11L19-N13	3
Caelo	Glucose monohydrate	12284202	6
Caelo	Glucose monohydrate	12284204	2
Caelo	Glucose monohydrate	12284206	6

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glucose monohydrate	12284219	8
Caelo	Glucose monohydrate	12284222	3
Caelo	Glucose monohydrate	12284229	3
Caelo	Glucose monohydrate	12284230	3
Caelo	Glucose monohydrate	12284231	1
Caelo	Glucose monohydrate	12345	1
Caelo	Glucose monohydrate	123456	2
Caelo	Glucose monohydrate	12435	1
Caelo	Glucose monohydrate	12G30-N01	1
Caelo	Glucose monohydrate	12G30-NO01	1
Caelo	Glucose monohydrate	1305030-02	1
Caelo	Glucose monohydrate	13157002	2
Caelo	Glucose monohydrate	13157004	1
Caelo	Glucose monohydrate	13157005	12
Caelo	Glucose monohydrate	13157007	6
Caelo	Glucose monohydrate	13157008	1
Caelo	Glucose monohydrate	13157011	9
Caelo	Glucose monohydrate	13157012	1
Caelo	Glucose monohydrate	13157013	1
Caelo	Glucose monohydrate	13157017	1
Caelo	Glucose monohydrate	13157019	10
Caelo	Glucose monohydrate	13157022	1
Caelo	Glucose monohydrate	13157026	3
Caelo	Glucose monohydrate	13A25-N01	5
Caelo	Glucose monohydrate	13H06-N08	2
Caelo	Glucose monohydrate	1410019-02	1
Caelo	Glucose monohydrate	14102401	4
Caelo	Glucose monohydrate	14102407	2
Caelo	Glucose monohydrate	14102411	4
Caelo	Glucose monohydrate	14102412	7
Caelo	Glucose monohydrate	14102415	2
Caelo	Glucose monohydrate	14102416	5
Caelo	Glucose monohydrate	14102418	10
Caelo	Glucose monohydrate	14102420	6
Caelo	Glucose monohydrate	14102421	4
Caelo	Glucose monohydrate	14102424	1
Caelo	Glucose monohydrate	14102427	1
Caelo	Glucose monohydrate	14102430	3
Caelo	Glucose monohydrate	14334802	11
Caelo	Glucose monohydrate	14334805	2
Caelo	Glucose monohydrate	14334806	3
Caelo	Glucose monohydrate	14334807	4
Caelo	Glucose monohydrate	14334808	2
Caelo	Glucose monohydrate	14334809	1
Caelo	Glucose monohydrate	14334810	8
Caelo	Glucose monohydrate	14334811	2
Caelo	Glucose monohydrate	14B04-B01-291137	1
Caelo	Glucose monohydrate	14B28-B02-291354	1
Caelo	Glucose monohydrate	14I04-B08	4
Caelo	Glucose monohydrate	150302G	1
Caelo	Glucose monohydrate	15095601	9
Caelo	Glucose monohydrate	15095602	1
Caelo	Glucose monohydrate	15095603	1
Caelo	Glucose monohydrate	15095605	3
Caelo	Glucose monohydrate	15095606	1
Caelo	Glucose monohydrate	15095611	3
Caelo	Glucose monohydrate	15095612	13
Caelo	Glucose monohydrate	15180001	12
Caelo	Glucose monohydrate	15180002	17
Caelo	Glucose monohydrate	15180003	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glucose monohydrate	15180005	3
Caelo	Glucose monohydrate	15180009	1
Caelo	Glucose monohydrate	15180010	8
Caelo	Glucose monohydrate	15180012	18
Caelo	Glucose monohydrate	15180013	2
Caelo	Glucose monohydrate	15180015	8
Caelo	Glucose monohydrate	15180016	2
Caelo	Glucose monohydrate	1518002	1
Caelo	Glucose monohydrate	15413301	1
Caelo	Glucose monohydrate	15413302	3
Caelo	Glucose monohydrate	15413303	1
Caelo	Glucose monohydrate	15413304	27
Caelo	Glucose monohydrate	15413304/20160309/6	1
Caelo	Glucose monohydrate	15413401	6
Caelo	Glucose monohydrate	15413402	6
Caelo	Glucose monohydrate	15413405	6
Caelo	Glucose monohydrate	15413409	25
Caelo	Glucose monohydrate	15413410	3
Caelo	Glucose monohydrate	15413412	3
Caelo	Glucose monohydrate	15413413	1
Caelo	Glucose monohydrate	154134o2	1
Caelo	Glucose monohydrate	160101	1
Caelo	Glucose monohydrate	160400601	1
Caelo	Glucose monohydrate	1604006-01	1
Caelo	Glucose monohydrate	1604104	1
Caelo	Glucose monohydrate	16049101	19
Caelo	Glucose monohydrate	16049102	9
Caelo	Glucose monohydrate	16049103	6
Caelo	Glucose monohydrate	16049104	19
Caelo	Glucose monohydrate	16049105	10
Caelo	Glucose monohydrate	16049107	6
Caelo	Glucose monohydrate	16049108	4
Caelo	Glucose monohydrate	1607024-01	1
Caelo	Glucose monohydrate	1618401	2
Caelo	Glucose monohydrate	16184616	1
Caelo	Glucose monohydrate	16184801	20
Caelo	Glucose monohydrate	16184802	2
Caelo	Glucose monohydrate	16184807	12
Caelo	Glucose monohydrate	16184808	6
Caelo	Glucose monohydrate	16184810	26
Caelo	Glucose monohydrate	16184816	3
Caelo	Glucose monohydrate	17005801	3
Caelo	Glucose monohydrate	17005802	12
Caelo	Glucose monohydrate	170058025312	1
Caelo	Glucose monohydrate	170058025458	1
Caelo	Glucose monohydrate	170058025517	1
Caelo	Glucose monohydrate	170058025621	1
Caelo	Glucose monohydrate	17005803	33
Caelo	Glucose monohydrate	17005804	10
Caelo	Glucose monohydrate	17005805	2
Caelo	Glucose monohydrate	17005811	2
Caelo	Glucose monohydrate	17005812	13
Caelo	Glucose monohydrate	17005813	7
Caelo	Glucose monohydrate	1701002-01	2
Caelo	Glucose monohydrate	170100401	1
Caelo	Glucose monohydrate	170323183	1
Caelo	Glucose monohydrate	1707004-001	1
Caelo	Glucose monohydrate	1707004-01	7
Caelo	Glucose monohydrate	17136801	31
Caelo	Glucose monohydrate	17136801/P-11101722	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glucose monohydrate	17136802	17
Caelo	Glucose monohydrate	17136804	20
Caelo	Glucose monohydrate	17136804x2	1
Caelo	Glucose monohydrate	17136805	14
Caelo	Glucose monohydrate	17305003	47
Caelo	Glucose monohydrate	17305004	13
Caelo	Glucose monohydrate	1801009	1
Caelo	Glucose monohydrate	1801009-01	4
Caelo	Glucose monohydrate	180101901	1
Caelo	Glucose monohydrate	180101907	1
Caelo	Glucose monohydrate	180300004	1
Caelo	Glucose monohydrate	18030003	15
Caelo	Glucose monohydrate	18030004	7
Caelo	Glucose monohydrate	18030005	7
Caelo	Glucose monohydrate	18030006	1
Caelo	Glucose monohydrate	1803006	1
Caelo	Glucose monohydrate	18064912	1
Caelo	Glucose monohydrate	180700501	1
Caelo	Glucose monohydrate	1807005-01	2
Caelo	Glucose monohydrate	1807005-02	1
Caelo	Glucose monohydrate	18071402	1
Caelo	Glucose monohydrate	18101901	67
Caelo	Glucose monohydrate	18101902	6
Caelo	Glucose monohydrate	18101903	24
Caelo	Glucose monohydrate	181019030	1
Caelo	Glucose monohydrate	18101907	34
Caelo	Glucose monohydrate	18101909	1
Caelo	Glucose monohydrate	18107907	1
Caelo	Glucose monohydrate	1810901	1
Caelo	Glucose monohydrate	1810907	1
Caelo	Glucose monohydrate	1811020-01	5
Caelo	Glucose monohydrate	181197	1
Caelo	Glucose monohydrate	181401903	1
Caelo	Glucose monohydrate	18214701	22
Caelo	Glucose monohydrate	18214702	1
Caelo	Glucose monohydrate	18214703	54
Caelo	Glucose monohydrate	18214704	20
Caelo	Glucose monohydrate	18214708	31
Caelo	Glucose monohydrate	18214709	5
Caelo	Glucose monohydrate	18214710	8
Caelo	Glucose monohydrate	18214712	1
Caelo	Glucose monohydrate	182414703	1
Caelo	Glucose monohydrate	1891009-01	1
Caelo	Glucose monohydrate	190073303	1
Caelo	Glucose monohydrate	190402901	1
Caelo	Glucose monohydrate	19073033	1
Caelo	Glucose monohydrate	19073301	12
Caelo	Glucose monohydrate	19073302	12
Caelo	Glucose monohydrate	190733023	1
Caelo	Glucose monohydrate	19073303	78
Caelo	Glucose monohydrate	19073304	18
Caelo	Glucose monohydrate	19073305	10
Caelo	Glucose monohydrate	19073309	29
Caelo	Glucose monohydrate	19073310	7
Caelo	Glucose monohydrate	190801201	2
Caelo	Glucose monohydrate	191486003	1
Caelo	Glucose monohydrate	19248600	1
Caelo	Glucose monohydrate	192486002	17
Caelo	Glucose monohydrate	192486003	68
Caelo	Glucose monohydrate	192486004	25

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glucose monohydrate	192486006	13
Caelo	Glucose monohydrate	192486007	9
Caelo	Glucose monohydrate	1973303	1
Caelo	Glucose monohydrate	200002144002	2
Caelo	Glucose monohydrate	2000214006	1
Caelo	Glucose monohydrate	20002144002	70
Caelo	Glucose monohydrate	20002144005	6
Caelo	Glucose monohydrate	20002144006	6
Caelo	Glucose monohydrate	20002144007	7
Caelo	Glucose monohydrate	20002144022	1
Caelo	Glucose monohydrate	200021444005	1
Caelo	Glucose monohydrate	20003963001	2
Caelo	Glucose monohydrate	20003964001	8
Caelo	Glucose monohydrate	20003964002	52
Caelo	Glucose monohydrate	20003964004	18
Caelo	Glucose monohydrate	20003964005	3
Caelo	Glucose monohydrate	20003964008	4
Caelo	Glucose monohydrate	20003964009	21
Caelo	Glucose monohydrate	20003964012	1
Caelo	Glucose monohydrate	20003964013	7
Caelo	Glucose monohydrate	20003964015	14
Caelo	Glucose monohydrate	20003964016	2
Caelo	Glucose monohydrate	20004180002	1
Caelo	Glucose monohydrate	2000418009	1
Caelo	Glucose monohydrate	200041820009	3
Caelo	Glucose monohydrate	20004182001	4
Caelo	Glucose monohydrate	20004182002	9
Caelo	Glucose monohydrate	20004182003	21
Caelo	Glucose monohydrate	20004182004	2
Caelo	Glucose monohydrate	20004182006	1
Caelo	Glucose monohydrate	20004182007	3
Caelo	Glucose monohydrate	20004182008	18
Caelo	Glucose monohydrate	20004182009	28
Caelo	Glucose monohydrate	20004182010	3
Caelo	Glucose monohydrate	2000418209	2
Caelo	Glucose monohydrate	2002144002	2
Caelo	Glucose monohydrate	2002144006	1
Caelo	Glucose monohydrate	200415PJK01	1
Caelo	Glucose monohydrate	2004182006	1
Caelo	Glucose monohydrate	2004182009	1
Caelo	Glucose monohydrate	2006007-01	2
Caelo	Glucose monohydrate	2009024-01	1
Caelo	Glucose monohydrate	2017Q-02209	1
Caelo	Glucose monohydrate	210018586004	1
Caelo	Glucose monohydrate	210018860008	3
Caelo	Glucose monohydrate	21001886003	10
Caelo	Glucose monohydrate	21001886004	25
Caelo	Glucose monohydrate	21001886005	19
Caelo	Glucose monohydrate	21001886008	5
Caelo	Glucose monohydrate	21001886009	9
Caelo	Glucose monohydrate	21001886011	6
Caelo	Glucose monohydrate	21001886013	2
Caelo	Glucose monohydrate	21002018013	1
Caelo	Glucose monohydrate	21004018003	6
Caelo	Glucose monohydrate	21004018006	5
Caelo	Glucose monohydrate	21004018007	16
Caelo	Glucose monohydrate	21004018009	6
Caelo	Glucose monohydrate	21004018011	1
Caelo	Glucose monohydrate	21004018013	5
Caelo	Glucose monohydrate	21004018014	18

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glucose monohydrate	21004018015	19
Caelo	Glucose monohydrate	21004018017	2
Caelo	Glucose monohydrate	21004018018	1
Caelo	Glucose monohydrate	2100886013	1
Caelo	Glucose monohydrate	2101402	1
Caelo	Glucose monohydrate	2103027-01	3
Caelo	Glucose monohydrate	2104018009	2
Caelo	Glucose monohydrate	219317005803	1
Caelo	Glucose monohydrate	22000456006	1
Caelo	Glucose monohydrate	22000756003	2
Caelo	Glucose monohydrate	22000756005	3
Caelo	Glucose monohydrate	22000756006	19
Caelo	Glucose monohydrate	22000756007	4
Caelo	Glucose monohydrate	22000756009	1
Caelo	Glucose monohydrate	22000756010	2
Caelo	Glucose monohydrate	22000756011	2
Caelo	Glucose monohydrate	22000756014	2
Caelo	Glucose monohydrate	22000756015	28
Caelo	Glucose monohydrate	22000756018	3
Caelo	Glucose monohydrate	22000756019	1
Caelo	Glucose monohydrate	22000756020	1
Caelo	Glucose monohydrate	22000756021	2
Caelo	Glucose monohydrate	22000756022	3
Caelo	Glucose monohydrate	220007567	1
Caelo	Glucose monohydrate	22001899002	3
Caelo	Glucose monohydrate	22001899003	1
Caelo	Glucose monohydrate	22001899005c	1
Caelo	Glucose monohydrate	220616(21004018009)	1
Caelo	Glucose monohydrate	220756015	1
Caelo	Glucose monohydrate	2222222222	1
Caelo	Glucose monohydrate	23000211004	3
Caelo	Glucose monohydrate	23000211008	1
Caelo	Glucose monohydrate	2300021104	1
Caelo	Glucose monohydrate	23051801	1
Caelo	Glucose monohydrate	2315Q-02209NP	1
Caelo	Glucose monohydrate	2316E-02209	1
Caelo	Glucose monohydrate	24081801	1
Caelo	Glucose monohydrate	26061802	1
Caelo	Glucose monohydrate	27081801	1
Caelo	Glucose monohydrate	2743	1
Caelo	Glucose monohydrate	2745	1
Caelo	Glucose monohydrate	2795	1
Caelo	Glucose monohydrate	28051507	1
Caelo	Glucose monohydrate	3612J-02209	1
Caelo	Glucose monohydrate	4616M-02209	1
Caelo	Glucose monohydrate	5051401	1
Caelo	Glucose monohydrate	5092	1
Caelo	Glucose monohydrate	613011-3p	1
Caelo	Glucose monohydrate	716I-02209	1
Caelo	Glucose monohydrate	718A-02209	1
Caelo	Glucose monohydrate	719092G	1
Caelo	Glucose monohydrate	72714068	1
Caelo	Glucose monohydrate	8697	1
Caelo	Glucose monohydrate	E144C	1
Caelo	Glucose monohydrate	E388S	1
Caelo	Glucose monohydrate	Test	1
Caelo	Glucose monohydrate	UIUJHJH	1
Caeo	Glucose monohydrate	1049103	1
Caeolo / noweda	Glucose monohydrate		1
Caeolo/Noweda	Glucose monohydrate	15413301	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caeolo/Phönix	Glucose monohydrate	16184810	2
Caesa/Phoenix	Glucose monohydrate	15413304	1
Caesar & Lorenz	Glucose monohydrate	13157007	1
Caesar & Loretz / Gehe	Glucose monohydrate	18214703	3
Caesar & Loretz GmbH...	Glucose monohydrate	19073305	1
Caesar & Loretz GmbH...	Glucose monohydrate	19073310	3
Caesar & Loretz GmbH...	Glucose monohydrate	19073303	2
Caesar & Loretz GmbH...	Glucose monohydrate	19073309	2
Caesar & Loretz GmbH...	Glucose monohydrate	192486003	3
Caesar & Loretz GmbH...	Glucose monohydrate	20003964002	1
Caesar & Loretz GmbH...	Glucose monohydrate	192486006	2
Caesar & Loretz GmbH...	Glucose monohydrate	20003964001	1
Caesar & Loretz GmbH...	Glucose monohydrate	20004182001	1
Caesar & Loretz GmbH...	Glucose monohydrate	21001886008	2
Caesar & Loretz GmbH...	Glucose monohydrate	21004018006	1
Caesar & Loretz GmbH...	Glucose monohydrate	21004018016	4
Caesar & Loretz GmbH...	Glucose monohydrate	21004018017	1
Caesar & Loretz GmbH...	Glucose monohydrate	22000756012	1
Caesar & Loretz GmbH...	Glucose monohydrate	192486007	3
Caesar & Loretz GmbH...	Glucose monohydrate	20003964008	1
Caesar & Loretz GmbH...	Glucose monohydrate	20004182006	1
Caesar & Loretz GmbH...	Glucose monohydrate	21001886003	1
Caesar & Loretz GmbH...	Glucose monohydrate	18214703	3
Caesar & Loretz GmbH L 50	Glucose monohydrate	22000756006	2
Caesar & Loretz GmbH...	Glucose monohydrate	21001886008	1
Caesar & Loretz GmbH...	Glucose monohydrate	20003964009	2
Caesar & Loretz GmbH...	Glucose monohydrate	21004018009	1
Caesar & Loretz GmbH/AEP	Glucose monohydrate	18214703	1
Caesar & Loretz GmbH/AEP	Glucose monohydrate	192486004	6
Caesar & Loretz GmbH/AHD	Glucose monohydrate	22000756004	1
Caesar & Loretz GmbH/AHD	Glucose monohydrate	22000756022	1
Caesar & Loretz GmbH...	Glucose monohydrate	192486002	2
Caesar & Loretz GmbH...	Glucose monohydrate	19073310	1
Caesar & Loretz GmbH...	Glucose monohydrate	192486007	1
Caesar & Loretz GmbH...	Glucose monohydrate	192486003	3
Caesar & Loretz GmbH...	Glucose monohydrate	20002144002	1
Caesar & Loretz GmbH/G	Glucose monohydrate	20003964002	1
Caesar & Loretz GmbH/Gehe	Glucose monohydrate	192486003	1
Caesar & Loretz GmbH/Gehe	Glucose monohydrate	20002144002	1
Caesar & Loretz GmbH/Gehe	Glucose monohydrate	20004182008	1
Caesar & Loretz GmbH/Gehe	Glucose monohydrate	21004018006	1
Caesar & Loretz GmbH...	Glucose monohydrate	20002144005	1
Caesar & Loretz GmbH/Gö	Glucose monohydrate	20002144002	1
Caesar & Loretz GmbH...	Glucose monohydrate	20002144002	1
Caesar & Loretz GmbH...	Glucose monohydrate	2009024-01	1
Caesar & Loretz GmbH/K	Glucose monohydrate	21004018014	1
Caesar & Loretz GmbH/Kehr	Glucose monohydrate	18214704	1
Caesar & Loretz GmbH...	Glucose monohydrate	20002144002	4
Caesar & Loretz GmbH...	Glucose monohydrate	20003964015	1
Caesar & Loretz GmbH...	Glucose monohydrate	20004182009	4
Caesar & Loretz GmbH/L10	Glucose monohydrate	21004018015	1
Caesar & Loretz GmbH...	Glucose monohydrate	19073303	3
Caesar & Loretz GmbH...	Glucose monohydrate	20004182008	2
Caesar & Loretz GmbH...	Glucose monohydrate	20004182003	2
Caesar & Loretz GmbH...	Glucose monohydrate	20004182006	1
Caesar & Loretz GmbH...	Glucose monohydrate	21001886008	1
Caesar & Loretz GmbH...	Glucose monohydrate	21004018009	2
Caesar & Loretz GmbH...	Glucose monohydrate	22001899001	1
Caesar & Loretz GmbH...	Glucose monohydrate	19073303	1
Caesar & Loretz GmbH...	Glucose monohydrate	19073309	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Glucose monohydrate	20003964002	5
Caesar & Loretz GmbH...	Glucose monohydrate	20003964009	3
Caesar & Loretz GmbH...	Glucose monohydrate	20004182009	2
Caesar & Loretz GmbH...	Glucose monohydrate	21004018007	1
Caesar & Loretz GmbH...	Glucose monohydrate	21004018015	1
Caesar & Loretz GmbH...	Glucose monohydrate	22000756006	1
Caesar & Loretz GmbH...	Glucose monohydrate	22000756006	2
Caesar & Loretz GmbH...	Glucose monohydrate	22000756015	2
Caesar & Loretz GmbH...	Glucose monohydrate	22001899005	2
Caesar & Loretz GmbH...	Glucose monohydrate	20002144002	1
Caesar & Loretz GmbH...	Glucose monohydrate	20003964002	1
Caesar & Loretz GmbH...	Glucose monohydrate	20003964004	1
Caesar & Loretz GmbH...	Glucose monohydrate	20004182003	1
Caesar & Loretz GmbH...	Glucose monohydrate	21001886004	1
Caesar & Loretz GmbH	Glucose monohydrate	128214703	1
Caesar & Loretz GmbH	Glucose monohydrate	15180010	1
Caesar & Loretz GmbH	Glucose monohydrate	15180013	1
Caesar & Loretz GmbH	Glucose monohydrate	15413402	1
Caesar & Loretz GmbH	Glucose monohydrate	17005802	1
Caesar & Loretz GmbH	Glucose monohydrate	18101901	1
Caesar & Loretz GmbH	Glucose monohydrate	18101907	3
Caesar & Loretz GmbH	Glucose monohydrate	18179716	1
Caesar & Loretz GmbH	Glucose monohydrate	18214701	1
Caesar & Loretz GmbH	Glucose monohydrate	18214703	19
Caesar & Loretz GmbH	Glucose monohydrate	18214704	2
Caesar & Loretz GmbH	Glucose monohydrate	18214708	5
Caesar & Loretz GmbH	Glucose monohydrate	18214710	1
Caesar & Loretz GmbH	Glucose monohydrate	19073301	1
Caesar & Loretz GmbH	Glucose monohydrate	19073302	3
Caesar & Loretz GmbH	Glucose monohydrate	19073303	24
Caesar & Loretz GmbH	Glucose monohydrate	19073304	10
Caesar & Loretz GmbH	Glucose monohydrate	19073305	1
Caesar & Loretz GmbH	Glucose monohydrate	19073309	8
Caesar & Loretz GmbH	Glucose monohydrate	19073310	5
Caesar & Loretz GmbH	Glucose monohydrate	192486002	5
Caesar & Loretz GmbH	Glucose monohydrate	192486003	16
Caesar & Loretz GmbH	Glucose monohydrate	192486004	4
Caesar & Loretz GmbH	Glucose monohydrate	192486006	3
Caesar & Loretz GmbH	Glucose monohydrate	192486007	1
Caesar & Loretz GmbH	Glucose monohydrate	20000461007	1
Caesar & Loretz GmbH	Glucose monohydrate	20002144002	7
CAESAR & LORETZ GMBH	Glucose monohydrate	20002144002	4
Caesar & Loretz GmbH	Glucose monohydrate	20002144005	1
Caesar & Loretz GmbH	Glucose monohydrate	20002144006	7
Caesar & Loretz GmbH	Glucose monohydrate	20002144007	2
Caesar & Loretz GmbH	Glucose monohydrate	20003963001	4
Caesar & Loretz GmbH	Glucose monohydrate	20003964001	2
Caesar & Loretz GmbH	Glucose monohydrate	20003964002	18
Caesar & Loretz GmbH	Glucose monohydrate	20003964004	3
Caesar & Loretz GmbH	Glucose monohydrate	20003964005	4
Caesar & Loretz GmbH	Glucose monohydrate	20003964008	1
Caesar & Loretz GmbH	Glucose monohydrate	20003964009	9
Caesar & Loretz GmbH	Glucose monohydrate	20003964012	6
Caesar & Loretz GmbH	Glucose monohydrate	20003964013	1
Caesar & Loretz GmbH	Glucose monohydrate	20003964015	4
Caesar & Loretz GmbH	Glucose monohydrate	20003964016	4
Caesar & Loretz GmbH	Glucose monohydrate	20004182001	2
Caesar & Loretz GmbH	Glucose monohydrate	20004182002	11
Caesar & Loretz GmbH	Glucose monohydrate	20004182003	10
Caesar & Loretz GmbH	Glucose monohydrate	20004182004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Glucose monohydrate	20004182006	2
Caesar & Loretz GmbH	Glucose monohydrate	20004182007	2
Caesar & Loretz GmbH	Glucose monohydrate	20004182008	9
Caesar & Loretz GmbH	Glucose monohydrate	20004182009	16
Caesar & Loretz GmbH	Glucose monohydrate	20004182010	1
Caesar & Loretz GmbH	Glucose monohydrate	2004182010	1
Caesar & Loretz GmbH	Glucose monohydrate	21001886003	1
Caesar & Loretz GmbH	Glucose monohydrate	21001886004	5
Caesar & Loretz GmbH	Glucose monohydrate	21001886005	16
CAESAR & LORETZ GMBH	Glucose monohydrate	21001886005	3
Caesar & Loretz GmbH	Glucose monohydrate	21001886008	3
Caesar & Loretz GmbH	Glucose monohydrate	21001886009	5
Caesar & Loretz GmbH	Glucose monohydrate	21001886011	3
Caesar & Loretz GmbH	Glucose monohydrate	21004018003	2
Caesar & Loretz GmbH	Glucose monohydrate	21004018006	3
Caesar & Loretz GmbH	Glucose monohydrate	21004018007	6
Caesar & Loretz GmbH	Glucose monohydrate	21004018009	2
Caesar & Loretz GmbH	Glucose monohydrate	21004018011	1
Caesar & Loretz GmbH	Glucose monohydrate	21004018013	1
Caesar & Loretz GmbH	Glucose monohydrate	21004018014	10
Caesar & Loretz GmbH	Glucose monohydrate	21004018015	9
Caesar & Loretz GmbH	Glucose monohydrate	2102027-1	1
Caesar & Loretz GmbH	Glucose monohydrate	22000756004	2
Caesar & Loretz GmbH	Glucose monohydrate	22000756006	5
Caesar & Loretz GmbH	Glucose monohydrate	22000756007	4
Caesar & Loretz GmbH	Glucose monohydrate	22000756009	1
Caesar & Loretz GmbH	Glucose monohydrate	22000756010	1
Caesar & Loretz GmbH	Glucose monohydrate	22000756011	1
Caesar & Loretz GmbH	Glucose monohydrate	22000756012	1
Caesar & Loretz GmbH	Glucose monohydrate	22000756013	1
Caesar & Loretz GmbH	Glucose monohydrate	22000756014	2
Caesar & Loretz GmbH	Glucose monohydrate	22000756015	21
Caesar & Loretz GmbH	Glucose monohydrate	22000756017	1
Caesar & Loretz GmbH	Glucose monohydrate	22000756018	1
Caesar & Loretz GmbH	Glucose monohydrate	22000756020	2
Caesar & Loretz GmbH	Glucose monohydrate	22000756021	1
Caesar & Loretz GmbH	Glucose monohydrate	22000756022	4
Caesar & Loretz GmbH	Glucose monohydrate	22001899001	3
Caesar & Loretz GmbH	Glucose monohydrate	22001899002	4
Caesar & Loretz GmbH	Glucose monohydrate	22001899010	1
Caesar & Loretz GmbH	Glucose monohydrate	22001899012	2
Caesar & Loretz GmbH	Glucose monohydrate	23000211001	1
Caesar & Loretz GmbHKehr	Glucose monohydrate	192486002	1
Caesar & Loretz/ Cae…	Glucose monohydrate	18030004	1
Caesar & Loretz/Noweda	Glucose monohydrate	16049102	1
Caesar & Loretz/Phönix	Glucose monohydrate	18101907	1
Caesar & Loretz	Glucose monohydrate	21001886008	1
Caesar & Loretz	Glucose monohydrate	22000756004	1
Caesar & Loretz	Glucose monohydrate	22000756010	1
Caesar / Gehe	Glucose monohydrate	17005802	1
Caesar und Loretz GmbH	Glucose monohydrate	16184807	1
Caesar&Loretz GmbH	Glucose monohydrate	22000756005	1
Caesar&Loretz GmbH	Glucose monohydrate	22000756009	1
Calo	Glucose monohydrate	15180010	2
Cealo/ Noweda	Glucose monohydrate	15413412	1
Cealo/Noweda	Glucose monohydrate	20003964012	2
Cealo/Sanacorp	Glucose monohydrate	22000756015	1
Cealo	Glucose monohydrate	13157017	1
Cealo	Glucose monohydrate	14102430	1
Celo/Jenne	Glucose monohydrate	20003964009	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Dermapharm	Glucose monohydrate	1601016-02	1
dextro energy / Noweda	Glucose monohydrate	L1299	1
Dextro Energy GmbH/Gehe	Glucose monohydrate	L4163	2
Dextro Energy GmbH/Gehe	Glucose monohydrate	L4164	1
Dextro Energy GmbH/Gehe	Glucose monohydrate	L4274	1
Dextro Energy GmbH/S...	Glucose monohydrate	L1299	1
Dextro Energy GmbH	Glucose monohydrate	5/2018L6315	1
Dextro energy/ Fiebig	Glucose monohydrate	L1147	1
Dextro Energy/Gehe	Glucose monohydrate	L1147	1
Dextro energy	Glucose monohydrate	L0086	1
Dextro energy	Glucose monohydrate	L0097	1
Dextro Energy	Glucose monohydrate	l3171	1
dextro energy	Glucose monohydrate	19016127	1
dextro energy	Glucose monohydrate	19050634	1
Dextro EnergyGmbH	Glucose monohydrate	L4036	1
Dextro EnergyGmbH	Glucose monohydrate	L4273	1
Dextro ernergy Gmbh	Glucose monohydrate	L6043	1
Dextro GmbH/Noweda	Glucose monohydrate	L5301	1
Dextro/Krieger/15.05.13	Glucose monohydrate	l3092	1
DextroEnergy/Noweda	Glucose monohydrate	L2283	1
dextroenergy	Glucose monohydrate	190161027	1
Dr. Aug. Wolff GmbH ...	Glucose monohydrate	21001886011	1
Eigenherstellung	Glucose monohydrate	110912HML01	1
Eigenherstellung	Glucose monohydrate	110913HJK02	1
Eigenherstellung	Glucose monohydrate	120912HML02	1
Eigenherstellung	Glucose monohydrate	160915HML01	1
Eigenherstellung	Glucose monohydrate	180213HJK01	1
Eigenherstellung	Glucose monohydrate	30912HML01	1
Eigenherstellung	Glucose monohydrate	40615HJK01	1
Eurho / Alliance	Glucose monohydrate	2001006-01	2
EuRho / Alliance	Glucose monohydrate	2103027-01	1
EuRho Noweda	Glucose monohydrate	2006007-01	1
EuRho/ Kehr	Glucose monohydrate	220201501	1
EuRho/Gehe 09.07.2022	Glucose monohydrate	2202015-01	1
EuRho/GEHE	Glucose monohydrate	1410019-01	1
EuRho/GEHE	Glucose monohydrate	1904029-01	2
EuRho/Noweda	Glucose monohydrate	2103027-01	7
EuRho/Phoenix	Glucose monohydrate	140500401	1
EuRho/Phoenix	Glucose monohydrate	1604006-01	1
EuRho/Phoenix	Glucose monohydrate	221005-02	1
Eurho/Sanacorp	Glucose monohydrate	1108061-01	2
EuRho	Glucose monohydrate	1108061-01	2
EuRho	Glucose monohydrate	1108061-02	1
EuRho	Glucose monohydrate	1204044-01	2
EuRho	Glucose monohydrate	151780	1
EuRho	Glucose monohydrate	1604006-0104932048	1
EuRho	Glucose monohydrate	1707004-01	2
EuRho	Glucose monohydrate	2006007-01	1
EuRho	Glucose monohydrate	2103027-01	1
EuRho	Glucose monohydrate	2710Q-02209	1
Euro OT>C	Glucose monohydrate	2006007-01	2
Euro OTC	Glucose monohydrate		1
Euro OTC	Glucose monohydrate	103027-012	3
Euro OTC	Glucose monohydrate	1103027-01	1
Euro OTC	Glucose monohydrate	1108061-01	2
Euro OTC	Glucose monohydrate	1114U2209	1
Euro OTC	Glucose monohydrate	1204044-01	3
Euro OTC	Glucose monohydrate	1204044-02	3
Euro OTC	Glucose monohydrate	1210034-01	9
Euro OTC	Glucose monohydrate	1210034-02	10

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Glucose monohydrate	1210034-03	1
Euro OTC	Glucose monohydrate	130503001	1
Euro OTC	Glucose monohydrate	1305030-01	6
Euro OTC	Glucose monohydrate	1305030-02	6
Euro OTC	Glucose monohydrate	1305030-02	1
Euro OTC	Glucose monohydrate	140004-01	1
Euro OTC	Glucose monohydrate	14005004-02	1
Euro OTC	Glucose monohydrate	140101901	1
Euro OTC	Glucose monohydrate	1401019-01	15
Euro OTC	Glucose monohydrate	140101902	2
Euro OTC	Glucose monohydrate	140500401	1
Euro OTC	Glucose monohydrate	1405004-01	16
Euro OTC	Glucose monohydrate	140500402	1
Euro OTC	Glucose monohydrate	1405004-02	4
Euro OTC	Glucose monohydrate	1406212209	1
Euro OTC	Glucose monohydrate	141001901	1
Euro OTC	Glucose monohydrate	1410019-01	7
Euro OTC	Glucose monohydrate	1410019-02	4
Euro OTC	Glucose monohydrate	150402801	1
Euro OTC	Glucose monohydrate	1504028-01	14
Euro OTC	Glucose monohydrate	1504028-02	10
Euro OTC	Glucose monohydrate	15040281	1
Euro OTC	Glucose monohydrate	150900601	1
Euro OTC	Glucose monohydrate	1509006-01	19
Euro OTC	Glucose monohydrate	1509006-02	5
Euro OTC	Glucose monohydrate	1509006-1	1
Euro OTC	Glucose monohydrate	15095601	1
Euro OTC	Glucose monohydrate	151780	1
Euro OTC	Glucose monohydrate	15180010	1
Euro OTC	Glucose monohydrate	160101601	2
Euro OTC	Glucose monohydrate	1601016-01	23
Euro OTC	Glucose monohydrate	1601016-02	5
Euro OTC	Glucose monohydrate	16040060-01	1
Euro OTC	Glucose monohydrate	1604006-01	33
Euro OTC	Glucose monohydrate	160400602	2
Euro OTC	Glucose monohydrate	1604006-02	30
Euro OTC	Glucose monohydrate	1607024	1
Euro OTC	Glucose monohydrate	1607024-01	19
Euro OTC	Glucose monohydrate	1607024-02	31
Euro OTC	Glucose monohydrate	160704-01	1
Euro OTC	Glucose monohydrate	16184807	1
Euro OTC	Glucose monohydrate	1701002_01	1
Euro OTC	Glucose monohydrate	1701002-01	29
Euro OTC	Glucose monohydrate	170100202	1
Euro OTC	Glucose monohydrate	1701002-02	7
Euro OTC	Glucose monohydrate	1707004	1
Euro OTC	Glucose monohydrate	1707004-001	1
Euro OTC	Glucose monohydrate	170700401	2
Euro OTC	Glucose monohydrate	1707004-01	69
Euro OTC	Glucose monohydrate	170704401	1
Euro OTC	Glucose monohydrate	17136801	1
Euro OTC	Glucose monohydrate	17136804	1
Euro OTC	Glucose monohydrate	180100-01	1
Euro OTC	Glucose monohydrate	1801009_01	1
Euro OTC	Glucose monohydrate	180100901	2
Euro OTC	Glucose monohydrate	1801009-01	75
Euro OTC	Glucose monohydrate	180100941	1
Euro OTC	Glucose monohydrate	18070005-001	1
Euro OTC	Glucose monohydrate	180700501	2
Euro OTC	Glucose monohydrate	1807005-01	45

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Glucose monohydrate	1807005-02	4
Euro OTC	Glucose monohydrate	18070501	1
Euro OTC	Glucose monohydrate	18070521	1
Euro OTC	Glucose monohydrate	18101901	2
Euro OTC	Glucose monohydrate	18101907	1
Euro OTC	Glucose monohydrate	181101001	1
Euro OTC	Glucose monohydrate	1811020	1
Euro OTC	Glucose monohydrate	181102001	2
Euro OTC	Glucose monohydrate	1811020-01	40
Euro OTC	Glucose monohydrate	1811020-02	8
Euro OTC	Glucose monohydrate	181102003	1
Euro OTC	Glucose monohydrate	1811020-1	1
Euro OTC	Glucose monohydrate	18110201-02	1
Euro OTC	Glucose monohydrate	18111020-01	1
Euro OTC	Glucose monohydrate	18214704	1
Euro OTC	Glucose monohydrate	187005-001	1
Euro OTC	Glucose monohydrate	1900402901	1
Euro OTC	Glucose monohydrate	1904029	1
Euro OTC	Glucose monohydrate	1904029/01	1
Euro OTC	Glucose monohydrate	190402901	4
Euro OTC	Glucose monohydrate	1904029-01	53
Euro OTC	Glucose monohydrate	190429-01	1
Euro OTC	Glucose monohydrate	1907012-01	1
Euro OTC	Glucose monohydrate	1908010-01	1
Euro OTC	Glucose monohydrate	1908012-01	56
Euro OTC	Glucose monohydrate	19080122-01	1
Euro OTC	Glucose monohydrate	190801241	1
Euro OTC	Glucose monohydrate	200007-01	1
Euro OTC	Glucose monohydrate	20009024-01	1
Euro OTC	Glucose monohydrate	2001006-001	1
Euro OTC	Glucose monohydrate	200100601	6
Euro OTC	Glucose monohydrate	2001006-01	67
Euro OTC	Glucose monohydrate	200600-01	1
Euro OTC	Glucose monohydrate	200600701	4
Euro OTC	Glucose monohydrate	2006007-01	48
Euro OTC	Glucose monohydrate	200902401	3
Euro OTC	Glucose monohydrate	2009024-01	105
Euro OTC	Glucose monohydrate	200902-41	1
Euro OTC	Glucose monohydrate	2013U-02209	1
Euro OTC	Glucose monohydrate	20160405-04	1
Euro OTC	Glucose monohydrate	2023012-1	1
Euro OTC	Glucose monohydrate	2103027	4
Euro OTC	Glucose monohydrate	210302701	2
Euro OTC	Glucose monohydrate	2103027-01	102
Euro OTC	Glucose monohydrate	210307-01	1
Euro OTC	Glucose monohydrate	2103207-01	1
Euro OTC	Glucose monohydrate	210327	1
Euro OTC	Glucose monohydrate	2107024_02	2
Euro OTC	Glucose monohydrate	2107024-01	29
Euro OTC	Glucose monohydrate	2107024-02	50
Euro OTC	Glucose monohydrate	2107042-02	1
Euro OTC	Glucose monohydrate	210724-02	1
Euro OTC	Glucose monohydrate	2109008	1
Euro OTC	Glucose monohydrate	2109008-01	33
Euro OTC	Glucose monohydrate	2109008-02	13
Euro OTC	Glucose monohydrate	219008-01	1
Euro OTC	Glucose monohydrate	2202015/01	1
Euro OTC	Glucose monohydrate	2202015-01	27
Euro OTC	Glucose monohydrate	2202015-02	30
Euro OTC	Glucose monohydrate	2202015-03	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Glucose monohydrate	22022015-01	1
Euro OTC	Glucose monohydrate	220601801	1
Euro OTC	Glucose monohydrate	2206018-01	46
Euro OTC	Glucose monohydrate	2206018-02	5
Euro OTC	Glucose monohydrate	2210005-01	5
Euro OTC	Glucose monohydrate	2210005-02	13
Euro OTC	Glucose monohydrate	226018-01	1
Euro OTC	Glucose monohydrate	2302007-01	3
Euro OTC	Glucose monohydrate	23051802	1
Euro OTC	Glucose monohydrate	2313E-02209	1
Euro OTC	Glucose monohydrate	31102013B	1
Euro OTC	Glucose monohydrate	8638943	1
Euro OTC	Glucose monohydrate	96-01	1
Euro OTC	Glucose monohydrate	E024R	1
Euro OTC	Glucose monohydrate	E042R/2009024-01	1
Euro OTC	Glucose monohydrate	E108T	3
Euro OTC	Glucose monohydrate	E255L	1
Euro OTC	Glucose monohydrate	E267X	1
Euro OTC	Glucose monohydrate	E388S	2
Euro OTC	Glucose monohydrate	E470S	2
Euro OTC	Glucose monohydrate	E617K	1
Euro OTC	Glucose monohydrate	E643N	1
Euro OTC	Glucose monohydrate	E732N	2
Euro OTC	Glucose monohydrate	E777P	2
Euro OTC	Glucose monohydrate	E882R	1
Euro OTC	Glucose monohydrate	E961M	1
Euro OTG/ AHD	Glucose monohydrate	1701002-01	1
Euro OTG/ AHD	Glucose monohydrate	1801009-01	1
Euro Pharma/Phönix	Glucose monohydrate	2103027-01	3
EuRo/ Noweda	Glucose monohydrate	1904029-01	1
Euro/ Sanacorp	Glucose monohydrate	1504028-01	1
Euro/Alliance Healthcare	Glucose monohydrate	1604006-01	1
Euro/Krieger	Glucose monohydrate	1807005-01	1
Euro/Noweda	Glucose monohydrate	1604006-02	2
Euro/Phoenix	Glucose monohydrate	210724-01	1
Euro/Phönix	Glucose monohydrate	1707004-01	1
Euro/Phönix	Glucose monohydrate	1811020-01	1
Euro/Phönix	Glucose monohydrate	1811020-02	1
Euro/Phönix	Glucose monohydrate	2210005-01	1
Euroo	Glucose monohydrate	1604006-01	1
Fagron	Glucose monohydrate		1
Fagron	Glucose monohydrate	11L19-N13	1
Fagron	Glucose monohydrate	12B09-N05	1
Fagron	Glucose monohydrate	12G30-N01	12
Fagron	Glucose monohydrate	12G30-NO1	2
Fagron	Glucose monohydrate	13A_N01	1
Fagron	Glucose monohydrate	13A25-n01	1
Fagron	Glucose monohydrate	13A25-N01	6
Fagron	Glucose monohydrate	13A25-No1	1
Fagron	Glucose monohydrate	13A25-NO1	2
Fagron	Glucose monohydrate	13B01-N03	5
Fagron	Glucose monohydrate	13C25N09	2
Fagron	Glucose monohydrate	13C25-N09	8
Fagron	Glucose monohydrate	13h06-n08	1
Fagron	Glucose monohydrate	13H06-N08	17
Fagron	Glucose monohydrate	13H14-B06-289483	1
Fagron	Glucose monohydrate	1401019-01	1
Fagron	Glucose monohydrate	1404-B08-298601	2
Fagron	Glucose monohydrate	1404-B08-298604	1
Fagron	Glucose monohydrate	1407-808-307707	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Glucose monohydrate	14102412	2
Fagron	Glucose monohydrate	14102420	1
Fagron	Glucose monohydrate	14104-B08-302707	1
Fagron	Glucose monohydrate	14B04-B01	3
Fagron	Glucose monohydrate	14B04-B01-291137	7
Fagron	Glucose monohydrate	14B04-B01-291138	3
Fagron	Glucose monohydrate	14B04-B01-291143	2
Fagron	Glucose monohydrate	14B28-B02	2
Fagron	Glucose monohydrate	14b28-b02-291353	1
Fagron	Glucose monohydrate	14B28-B02-291353	11
Fagron	Glucose monohydrate	14B28-B02-291354	3
Fagron	Glucose monohydrate	14D30-B06-294678	1
Fagron	Glucose monohydrate	14D30-bo6-294678	1
Fagron	Glucose monohydrate	14I04-808	1
Fagron	Glucose monohydrate	14I04-B08	1
Fagron	Glucose monohydrate	14I04-B08-298601	1
Fagron	Glucose monohydrate	14I04-B08-298602	3
Fagron	Glucose monohydrate	14I04B8298602	1
Fagron	Glucose monohydrate	1509006-01	1
Fagron	Glucose monohydrate	151780-0004	1
Fagron	Glucose monohydrate	1521-B06-309508	1
Fagron	Glucose monohydrate	15A21-B06-309508	3
Fagron	Glucose monohydrate	15B01291137	1
Fagron	Glucose monohydrate	17136805	1
Fagron	Glucose monohydrate	18101903	2
Fagron	Glucose monohydrate	270313PML01	1
Fagron	Glucose monohydrate	3413E-02209	1
Fagron	Glucose monohydrate	4213Q-02209	1
Fagron	Glucose monohydrate	4562135	1
Fagron	Glucose monohydrate	8G31-N09	1
Fagron	Glucose monohydrate	E0AJ5	1
Fagron	Glucose monohydrate	E144C	1
Fagron	Glucose monohydrate	E524W	1
Fagron	Glucose monohydrate	E571X	1
Fargon	Glucose monohydrate	13C25-N09	1
Fargron	Glucose monohydrate	13A25-N01	1
Fiebig/ Dextropur	Glucose monohydrate	L7045	1
Fiebig	Glucose monohydrate	18101907	1
Fragon	Glucose monohydrate	13H06-N08	1
Frey+Lau GmbH	Glucose monohydrate	1601016-01	1
GATT-KOLLER/PHOENIX	Glucose monohydrate	243/02141714	1
GATT-KOLLER/PHOENIX	Glucose monohydrate	243/02142614	1
Gehe	Glucose monohydrate	13157026	2
GEHE	Glucose monohydrate	17005803	1
Gehe	Glucose monohydrate	1707004-01	1
GEHE	Glucose monohydrate	1707004-01	1
Gehe	Glucose monohydrate	17305003	1
GEHE	Glucose monohydrate	18030003	2
Gehe	Glucose monohydrate	18101907	1
Gehe	Glucose monohydrate	18214703	1
Gehe	Glucose monohydrate	22001899011	4
Gehe	Glucose monohydrate	23000211001	1
Gehe	Glucose monohydrate	2302007-01	6
geibo	Glucose monohydrate	220601801	1
Gutenberg-Apotheke	Glucose monohydrate	14B04-B01	1
hzdjfdj	Glucose monohydrate	jdhdfhhf	1
Jenne	Glucose monohydrate	2009024-01	1
Jenne	Glucose monohydrate	22001899002	1
Jenne	Glucose monohydrate	2210005-02	2
Kehr	Glucose monohydrate	18101907	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Kehr	Glucose monohydrate	22000756019	1
Kehr	Glucose monohydrate	23000211010	1
Klenk	Glucose monohydrate	112233	1
Klosterring	Glucose monohydrate	17136802	1
Kyberg Experts	Glucose monohydrate	L9009	1
Mohrenapo	Glucose monohydrate	192486003	1
Noweda 10.02.2015	Glucose monohydrate	14334802	3
Noweda 10.032016	Glucose monohydrate	15413304	2
Noweda 30.07.2015	Glucose monohydrate	15095612	1
Noweda/apo-ident	Glucose monohydrate	210702402	1
Noweda/EuRho 01.02.2...	Glucose monohydrate	2009024-01	1
Noweda	Glucose monohydrate	1204044-01	2
Noweda	Glucose monohydrate	1210034	1
Noweda	Glucose monohydrate	151780	1
Noweda	Glucose monohydrate	1601016-01	1
Noweda	Glucose monohydrate	1607024-02	1
Noweda	Glucose monohydrate	17005801	1
Noweda	Glucose monohydrate	1701002-01	2
Noweda	Glucose monohydrate	1807005-01	1
Noweda	Glucose monohydrate	18101909	1
Noweda	Glucose monohydrate	1811020-02	1
Noweda	Glucose monohydrate	1904029-01	3
Noweda	Glucose monohydrate	1908012-01	2
Noweda	Glucose monohydrate	2006007-01E777P	1
Noweda	Glucose monohydrate	200902401	2
Noweda	Glucose monohydrate	2009024-01	1
Noweda	Glucose monohydrate	2107024-02	1
Noweda	Glucose monohydrate	22000756006	2
Noweda	Glucose monohydrate	22001899010	1
NOWEDA	Glucose monohydrate	2206018-01	1
Noweda	Glucose monohydrate	2210005-02	1
Noweda	Glucose monohydrate	2230756007	1
Noweda	Glucose monohydrate	A000018	1
Noweda	Glucose monohydrate	E882R	2
Pala	Glucose monohydrate	18214704	1
Pala	Glucose monohydrate	192486002	1
Ph.Eur.8.0	Glucose monohydrate	1401019-02	1
ph.Eur	Glucose monohydrate	2206018-01	1
pharma gmbh	Glucose monohydrate	1401019-01	1
Phoenix/Cealo	Glucose monohydrate	17305004	1
Phoenix	Glucose monohydrate	1707004-01	1
Phoenix	Glucose monohydrate	18101901	1
Phoenix	Glucose monohydrate	18214710	1
Phoenix	Glucose monohydrate	192486002	1
Phoenix	Glucose monohydrate	192486007	1
Phoenix	Glucose monohydrate	20003963001	1
Phoenix	Glucose monohydrate	2100186003	1
Phoenix	Glucose monohydrate	210702402	1
Phoenix	Glucose monohydrate	210800_01	1
Phoenix	Glucose monohydrate	22000756006	1
Phoenix	Glucose monohydrate	22000756019	1
Phoenix	Glucose monohydrate	2302007-01	2
Phoenix	Glucose monohydrate	3242	1
Phoenix	Glucose monohydrate	3385	1
Phönix Gotha	Glucose monohydrate	1401019-01	1
Phönix Gotha	Glucose monohydrate	1405004-02	1
Phönix Gotha	Glucose monohydrate	17136801	1
Phönix Gotha	Glucose monohydrate	17305003	1
Phönix Gotha	Glucose monohydrate	18101901	1
Phönix Gotha	Glucose monohydrate	18214703	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix Gotha	Glucose monohydrate	19073303	2
Phönix Gotha	Glucose monohydrate	192486003	1
Phönix	Glucose monohydrate	1210334-02	1
Phönix	Glucose monohydrate	1401019-01	1
phönix	Glucose monohydrate	16049101	1
phönix	Glucose monohydrate	16049104	1
phönix	Glucose monohydrate	16184816	1
Phönix	Glucose monohydrate	1801009-01	1
Phönix	Glucose monohydrate	18030005	1
Phönix	Glucose monohydrate	1807005-01	1
Phönix	Glucose monohydrate	18101901	2
Phönix	Glucose monohydrate	18101907	1
Phönix	Glucose monohydrate	18214703	1
Phönix	Glucose monohydrate	1904029-01	1
Phönix	Glucose monohydrate	19073304	1
Phönix	Glucose monohydrate	192486003	1
Phönix	Glucose monohydrate	200002144002	1
Phönix	Glucose monohydrate	20003963001	1
Phönix	Glucose monohydrate	20003964009	1
Phönix	Glucose monohydrate	20004182009	1
Phönix	Glucose monohydrate	200100601	1
Phönix	Glucose monohydrate	2006007-01	1
Phönix	Glucose monohydrate	21004018014	1
Phönix	Glucose monohydrate	22001899010	1
phönix	Glucose monohydrate	2202015-03	1
phönix	Glucose monohydrate	2206018-01	1
Phönix	Glucose monohydrate	23000211006	3
Phönix	Glucose monohydrate	23003430001	1
Roquette Freres/AHD	Glucose monohydrate	12G30-N01	1
Roquette Lestrem FR/…	Glucose monohydrate	1210034-02	1
Roquette Lestrem	Glucose monohydrate	160702402	1
Roquette Lestrem	Glucose monohydrate	1904029-01	8
roquette lestrem	Glucose monohydrate	2009024-01	2
Roquette/Phoenix	Glucose monohydrate	E732N	1
sana	Glucose monohydrate	15095601	2
Sanacop	Glucose monohydrate		1
Sanacorp,30.03.17, 7,12EUR	Glucose monohydrate	16184810	1
Sanacorp	Glucose monohydrate	12284230	1
sanacorp	Glucose monohydrate	13157026	1
Sanacorp	Glucose monohydrate	14102430	1
Sanacorp	Glucose monohydrate	1607024-01	1
Sanacorp	Glucose monohydrate	16184810	1
Sanacorp	Glucose monohydrate	17136804	1
Sanacorp	Glucose monohydrate	1807005-02	1
Sanacorp	Glucose monohydrate	18101903	2
Sanacorp	Glucose monohydrate	18101907	1
Sanacorp	Glucose monohydrate	1811020	1
Sanacorp	Glucose monohydrate	18214703	1
Sanacorp	Glucose monohydrate	18214704	1
Sanacorp	Glucose monohydrate	19073301	1
Sanacorp	Glucose monohydrate	19073303	1
sanacorp	Glucose monohydrate	19073304	1
Sanacorp	Glucose monohydrate	192486002	1
Sanacorp	Glucose monohydrate	20004182008	1
Sanacorp	Glucose monohydrate	2001006-01	1
Sanacorp	Glucose monohydrate	21001886009	1
sanacorp	Glucose monohydrate	2103027-01	1
Sanacorp	Glucose monohydrate	2107024-02	2
Sanacorp	Glucose monohydrate	22000756007	1
Sanacorp	Glucose monohydrate	22000756017	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Glucose monohydrate	2202015-01	1
Sanacorp	Glucose monohydrate	2206018-01	2
Sanacorp	Glucose monohydrate	23000211001	1
Sanacorp	Glucose monohydrate	23000211005	1
Sanacorp	Glucose monohydrate	2310008-01	1
Sanacorp	Glucose monohydrate	3/AKD100	1
Sanacorp	Glucose monohydrate	E316T	1
Sanacorp	Glucose monohydrate	E388S	2
sittig	Glucose monohydrate	17005805	1
Sonnenberg-Apotheke	Glucose monohydrate	140500401	1

- 231 534 spectra from 1515 *Apo-Ident* customers from a total of 48 694 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Glucose monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Glucose monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	520	0	152 442
Type B	0	970	0	201 114
Type C	0	4525	8	231 534

The substance/substance group *Glucose monohydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8462 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.3814 %)
Type C	100.0000 % (> 99.9007 %)	99.8235 % (> 99.7573 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20799	22538	5.99	167.74
21274	21905	6.28	171.69
21905	21905	0.00	165.89
22308	22308	0.00	169.89
22538	22538	0.00	168.50
23006	23006	0.00	167.90
23304	23304	0.00	168.92
23802	23802	0.00	171.02
24162	24162	0.00	173.37
25627	25627	0.00	171.05
25637	25637	0.00	170.23
25653	25653	0.00	170.65

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Glutamic acid**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20436-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Glutamic acid; Acidum glutaminicum

Special notes

When selecting the *Glutamic acid* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Glutamic acid	5	2	3

Second-stage model

For differentiation of the substance/substance group *Glutamic acid* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Glutamic acid* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Glycine	89.29	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Glutamic acid* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Glutamic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Glutamic acid	1604056	22562	40	20160523*
Euro OTC	Glutamic acid	1604056	24124	40	20180613*
Euro OTC	Glutamic acid	2002044	25158	40	20200513*
Euro OTC	Glutamic acid	2305025	26753	40	20230705*
Fagron	Glutamic acid	11I30-N02	20840	40	AR-15-FG-010446-02
Fagron	Glutamic acid	15G31-B08-311884	23599	40	20150817

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 6 reference samples from the substance/substance group *Glutamic acid*. These

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 722 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 100 spectra of 3 reference samples from the substance/substance group *Glutamic acid*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Glutamic acid	1907031	24788	40
Euro OTC	Glutamic acid	2008026	25405	40
Euro OTC	Glutamic acid	2305025	26753SI†	20

- 201 984 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Glutamic acid*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Glutamic acid	2008026-01	1
Euro OTC	Glutamic acid	28071505	1
Fagron	Glutamic acid	3031502	1

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 236 064 spectra from 1515 *Apo-Ident* customers from a total of 49 255 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Glutamic acid* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Glutamic acid* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	240	0	152 722
Type B	0	100	0	201 984
Type C	0	3	0	236 064

The substance/substance group *Glutamic acid* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.9011 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20840	20840	0.00	157.89
22562	22562	0.00	158.85
23599	22562	7.72	125.89
24124	24124	0.00	150.07
25158	25158	0.00	158.22
26753	26753	0.00	162.78

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Glutamine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	23150-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Glutamine; Glutaminum; L-glutamine

Special notes

When selecting the *Glutamine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Glutamine	6	7	1

Second-stage model

For differentiation of the substance/substance group *Glutamine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Glutamine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	113.88	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Glutamine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Glutamine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Glutamine	1702007	23150	40	20170322*
Euro OTC	Glutamine	1706010	23543	40	20170802*
Euro OTC	Glutamine	2003034	25238	40	20200619*
Euro OTC	Glutamine	2006029	25347	40	20200813*
Euro OTC	Glutamine	2011010	25458	40	20201208*
Fagron	Glutamine	17E05-B06-334869	23415	40	20170601
Fagron	Glutamine	17E05-B06-334869	23416	40	AR-17-FG-016178-01

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 280 spectra of 7 reference samples from the substance/substance group *Glutamine*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 682 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 330 spectra of 9 reference samples from the substance/substance group *Glutamine*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Glutamine	1802010	23950	40
Euro OTC	Glutamine	1806001	24121	40
Euro OTC	Glutamine	1901009	24483	40
Euro OTC	Glutamine	2101010	25576	40
Euro OTC	Glutamine	2108006	25773	50
Euro OTC	Glutamine	2205028	26224	40
Euro OTC	Glutamine	2301005	26519	40
Euro OTC	Glutamine	2205028	26224SI	20
Euro OTC	Glutamine	2301005	26519SI	20

- 201 754 spectra from a total of 4038 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Glutamine*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Glutamine	1706010-01	1

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Glutamine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Glutamine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	330	0	201 754
Type C	0	1	0	236 066

The substance/substance group *Glutamine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.1818 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23150	23150	0.00	205.25
23415	23416	1.74	211.62
23416	23416	0.00	211.34
23543	23543	0.00	204.82
25238	25238	0.00	205.77
25347	25347	0.00	208.49
25458	25458	0.00	210.93

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Glutathione**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20366-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Glutathione; Glutathionum

Special notes

When selecting the *Glutathione* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Glutathione	7	7	12

Second-stage model

For differentiation of the substance/substance group *Glutathione* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Glutathione* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	80.43	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Glutathione* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Glutathione*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Glutathione	1102019-02	21788	60	AR-15-FG-008218-01
Euro OTC	Glutathione	1703008	23143	40	20170327*
Euro OTC	Glutathione	1808036	24314	40	20180919*
Euro OTC	Glutathione	2002042	25250	40	20200622*
Euro OTC	Glutathione	2007021	25337	40	20200810*
Euro OTC	Glutathione	2306012	27069	40	20240208*
Euro OTC	Glutathione	2306012	27069SI	20	20240208*
Fagron	Glutathione	18C01-B08-347604	24059	40	20180416

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 320 spectra of 8 reference samples from the substance/substance group *Glutathione*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 642 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 300 spectra of 8 reference samples from the substance/substance group *Glutathione*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Glutathione	1711009	23729	40
Euro OTC	Glutathione	1901052	24491	40
Euro OTC	Glutathione	1905011	24675	40
Euro OTC	Glutathione	2105017	25680	40
Euro OTC	Glutathione	2205027	26436	40
Fagron	Glutathione	19B04-B04-365527	25439	40
Fagron	Glutathione	22K21-B03-230393	26978	40
Fagron	Glutathione	22K21-B03-230393	26978SI	20

- 201 784 spectra from a total of 4038 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 25 spectra from 5 *Apo-Ident* customers from 12 batches from the substance/substance group *Glutathione*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Changsha Huir	Glutathione	2201190	1
Euro OTC	Glutathione	1905011-01	1
Euro OTC	Glutathione	2002042-01	13
Fagron	Glutathione	14H21-B02	1
Farmalabor	Glutathione	P1700811	1
Shangei tengben Biot…	Glutathione	B210411	1
Vivatis Pharma	Glutathione	B200617	1
Vivatis Pharma	Glutathione	B210107	1
Vivatis Pharma	Glutathione	B210115	1
Vivatis Pharma	Glutathione	B210413	2
Vivatis Pharma	Glutathione	B210530	1
Vivatis Pharma	Glutathione	B220117	1

- 236 042 spectra from 1515 *Apo-Ident* customers from a total of 49 246 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Glutathione* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Glutathione* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	300	0	201 784
Type C	0	25	0	236 042

The substance/substance group *Glutathione* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 76.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21788	21788	0.00	165.93
23143	23143	0.00	170.71
24059	27069	8.46	174.74
24314	24314	0.00	148.28
25250	25250	0.00	160.54
25337	25337	0.00	163.28
27069	27069	0.00	167.08

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Glycine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20823-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Glycine; Glycinum

Special notes

When selecting the *Glycine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Glycine	11	16	15

Second-stage model

For differentiation of the substance/substance group *Glycine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Glycine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
L-alanine	101.64	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Glycine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Glycine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Glycine	13157303	21687	60	20130625
Caelo	Glycine	14147006	21818	60	AR-16-FG-012263-01
Caelo	Glycine	15262518	23124	40	20150910
Caelo	Glycine	170265	23295	40	20170315*
Caelo	Glycine	173493	23834	40	20180117*
Caelo	Glycine	20001656	25218	40	20200703*
Caelo	Glycine	22002518	26368	40	20220926*
Caelo	Glycine	22002518	26368SI	20	20220926*
Euro OTC	Glycine	1402022-01	21284	40	20140328
Euro OTC	Glycine	1402022-01	21534	60	AR-15-FG-005430-01
Euro OTC	Glycine	1801005	23912	40	20180125*
Fagron	Glycine	12G13-N04	20823	40	1401163
Fagron	Glycine	13G09-N03	21276	40	20120711

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 560 spectra of 13 reference samples from the substance/substance group *Glycine*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 402 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 710 spectra of 20 reference samples from the substance/substance group *Glycine*.

- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Glycine	191009	24507	40
Caelo	Glycine	23002306	26957	40
Caelo	Glycine	24001068	27319	40
Euro OTC	Glycine	1605035	22683	40
Euro OTC	Glycine	1704015	23387	40
Euro OTC	Glycine	1906006	24793	40
Euro OTC	Glycine	1911011	25103	40
Euro OTC	Glycine	2005028	25291	40
Euro OTC	Glycine	2009013	25424	40
Euro OTC	Glycine	2101030	25529	40
Euro OTC	Glycine	2203024	26038	40
Euro OTC	Glycine	2301025	26647	40
Euro OTC	Glycine	2307011	26890	40
Euro OTC	Glycine	2307010	26891	40
Euro OTC	Glycine	2404013	27364	40
Fagron	Glycine	23G05-B12-230974	26987	40
Caelo	Glycine	24001068	27319SI	20
Euro OTC	Glycine	2203024	26038SI	10
Euro OTC	Glycine	2301025	26647SI	20
Euro OTC	Glycine	2404013	27364SI	20

- 201 374 spectra from a total of 4029 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information

provided by the customer regarding manufacturer and batch number.

- 31 spectra from 13 *Apo-Ident* customers from 16 batches from the substance/substance group *Glycine*.
- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Glycine	14147005	1
Caelo	Glycine	15262502	2
Caelo	Glycine	15262503	1
Caelo	Glycine	15262504	1
Caelo	Glycine	15262518	1
Caelo	Glycine	17026502	1
Caelo	Glycine	19100902	3
Caesar & Loretz GmbH	Glycine	17349306	1
Caesar & Loretz GmbH	Glycine	19100902	2
Caesar & Loretz GmbH	Glycine	19100903	2
Euro OTC	Glycine	1801005-01	1
Euro OTC	Glycine	1906006-01	1
Euro OTC	Glycine	2101030-01	4
Euro OTC	Glycine	2203024-01	3
Fagron	Glycine	19E29-B04-366853	1
Fagron	Glycine	20J13-F06-374988	1
Fagron	Glycine	20J13-F06-376061	4
Sanacorp	Glycine	17349306	1

- 236 036 spectra from 1515 *Apo-Ident* customers from a total of 49 242 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Glycine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Glycine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	560	0	152 402
Type B	0	710	0	201 374
Type C	0	31	0	236 036

The substance/substance group *Glycine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9286 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.1549 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 80.6452 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20823	20823	0.00	196.73
21276	20823	13.50	198.73
21284	21534	13.20	182.97
21534	21534	0.00	179.85
21687	21534	15.31	184.83
21818	21818	0.00	213.08
23124	20823	31.44	193.55
23295	23295	0.00	210.67
23834	23834	0.00	184.08
23912	23912	0.00	181.20
25218	25218	0.00	205.90
26368	26368	0.00	183.62

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Glycopyrronium bromide**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	23076-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Glycopyrronium bromide; Glycopyrronii bromidum

Special notes

When selecting the *Glycopyrronium bromide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Glycopyrronium bromide	6	3	3

Second-stage model

For differentiation of the substance/substance group *Glycopyrronium bromide* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Glycopyrronium bromide* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Clobetasol propionate	111.74	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Glycopyrronium bromide* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Glycopyrronium bromide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Glycopyrronium bromide	16E09-B08-331027	23076	40	1707615
Fagron	Glycopyrronium bromide	16E09-B08-331027	23077	40	20160530
Fagron	Glycopyrronium bromide	18C30-B07-350744	24183	40	20180502
Fagron	Glycopyrronium bromide	18G25-B01-356318	24575	40	20180907
Fagron	Glycopyrronium bromide	20B03-F12-368270	25440	40	20200228
Fagron	Glycopyrronium bromide	22B10-B05-219477	26285	40	20220624
Fagron	Glycopyrronium bromide	23C02-B07-228663	26669	40	20230321

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 7 reference samples from the substance/substance group *Glycopyrronium bromide*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 682 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 6 reference samples from the substance/substance group *Glycopyrronium bromide*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Glycopyrronium bromide	17D28-B04-341606	23939	40
Fagron	Glycopyrronium bromide	21A08-F03-376481	25742	50
Fagron	Glycopyrronium bromide	21H13-B22-215731	25906	40
Fagron	Glycopyrronium bromide	21H13-B22-215731	25906SI	10
Fagron	Glycopyrronium bromide	22B10-B05-219477	26285SI†	20
Fagron	Glycopyrronium bromide	23C02-B07-228663	26669SI†	20

- 201 904 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 7 spectra from 6 *Apo-Ident* customers from 4 batches from the substance/substance group *Glycopyrronium bromide*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Fagron	Glycopyrronium bromide	18C30-B07-350744	3
Fagron	Glycopyrronium bromide	21A08-F03-376481	2
Fagron	Glycopyrronium bromide	21H13-B22-215731	1
Fagron	Glycopyrronium bromide	21H13-B22-217575	1

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 236 060 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Glycopyrronium bromide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Glycopyrronium bromide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	180	0	201 904
Type C	0	7	0	236 060

The substance/substance group *Glycopyrronium bromide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23076	23076	0.00	131.48
23077	23076	2.68	131.10
24183	23076	6.39	130.08
24575	23076	10.09	129.80
25440	23076	12.48	129.34
26285	23076	13.49	128.19
26669	23076	14.31	128.57

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Gramicidin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20203-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Gramicidin; Gramicidinum

Special notes

When selecting the *Gramicidin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Gramicidin	6	3	9

Second-stage model

For differentiation of the substance/substance group *Gramicidin* the following second-stage model is used:

- Submodel 02

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Gramicidin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	65.67	–
⋮	⋮	⋮
Tyrothricin	>50	52.43
Fluocinolone acetonide	>50	99.37
Methylprednisolone	>50	99.68
Triamcinolone acetonide	>50	104.32
Prednisolone	>50	125.28
Betamethasone	>50	165.20
Dexamethasone	>50	169.13

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Gramicidin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Gramicidin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Gramicidin	13J15-N02	21253	40	AR-15-FG-000813-01
Fagron	Gramicidin	17E09-B02-341211	23744	40	AR-18-FG-008970-02
Fagron	Gramicidin	18A19-B14-350428	24171	40	20180704
Fagron	Gramicidin	18L20-B01-358528	24571	40	20190320
Fagron	Gramicidin	19D30-B01-195185	25181	40	20190619
Fagron	Gramicidin	21G10-B12-213720	26326	40	20210928
Fagron	Gramicidin	21G10-B12-213720	26326SI	20	20210928

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 7 reference samples from the substance/substance group *Gramicidin*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Gramicidin*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Gramicidin	14C07-B06-292886	21544	40
Fagron	Gramicidin	15H18-B01-316269	22748	40
Fagron	Gramicidin	20I29-B07-200272	25587	40

- 201 964 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 12 spectra from 7 *Apo-Ident* customers from 11 batches from the substance/substance group *Gramicidin*.

- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Fagron	Gramicidin		1
Fagron	Gramicidin	11F-24-N03	1
Fagron	Gramicidin	12K22-N12	1
Fagron	Gramicidin	14H06-B03-297614	2
Fagron	Gramicidin	15C11-B04-306766	1
Fagron	Gramicidin	15H18B01316269	1
Fagron	Gramicidin	17E09-B02-341211	1
Fagron	Gramicidin	20129-B07-200272	1
Fagron	Gramicidin	20I29B07200272	1
Fagron	Gramicidin	21G10B12213720	1
Fagron	Gramicidin	B3200266	1

- 236 055 spectra from 1515 *Apo-Ident* customers from a total of 49 247 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Gramicidin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Gramicidin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	120	0	201 964
Type C	0	12	0	236 055

The substance/substance group *Gramicidin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21253	21253	0.00	114.94
23744	23744	0.00	118.00
24171	23744	4.74	117.96
24571	21253	9.12	128.15
25181	23744	4.93	124.45
26326	23744	6.15	125.34

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Griseofulvin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20939-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Griseofulvin; Griseofulvinum

Special notes

When selecting the *Griseofulvin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Griseofulvin	4	2	61

Second-stage model

For differentiation of the substance/substance group *Griseofulvin* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Griseofulvin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Neostigmine bromide	101.61	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Griseofulvin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Griseofulvin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Griseofulvin	13D19-N03	20939	40	1401419
Fagron	Griseofulvin	14E16-B01-296834	21725	60	20140526
Fagron	Griseofulvin	16F13-B06-330832	23594	40	20160713
Fagron	Griseofulvin	22K14-B07-213300	26459	40	20221123
Fagron	Griseofulvin	22K14-B07-213300	26459SI	20	20221123

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Griseofulvin*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 762 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Griseofulvin*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Griseofulvin	17L05-B05-345995	23996	40
Fagron	Griseofulvin	18L04_B01-357660	24440	40

- 202 004 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 134 spectra from 51 *Apo-Ident* customers from 67 batches from the substance/substance group *Griseofulvin*.
- Among them are spectra of independent samples from 61 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
AHD	Griseofulvin	17L05-B05-349129	1
AHD	Griseofulvin	18L04-B01-357660	1
AHD	Griseofulvin	18L04-B01-361614	1
AHD	Griseofulvin	18Lo4-B01-357660	1
AHD	Griseofulvin	B01-3616104	1
Alliance Healthcare	Griseofulvin	18L04-B01-363841	1
Bombastus	Griseofulvin	15L03-HH150640	1
Bombastus	Griseofulvin	16F13-B06-326073	1
Bombastus	Griseofulvin	17L05-B05-345996	1
Caelo	Griseofulvin	100910	1
Caelo	Griseofulvin	16F13-B06-323068	1
Caelo	Griseofulvin	16F13-B06-326074	1
Caelo	Griseofulvin	16F13-B06-330833	1
Euro OTC	Griseofulvin		1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Griseofulvin	14E16-B01-300367	1
Fagron	Griseofulvin	10F03-N12	1
Fagron	Griseofulvin	11J11-N13	1
Fagron	Griseofulvin	12D04-N12	1
Fagron	Griseofulvin	12F18-N04	1
Fagron	Griseofulvin	130922	2
Fagron	Griseofulvin	13D19-N03	1
Fagron	Griseofulvin	13F12-N22	1
Fagron	Griseofulvin	13L13-B08	1
Fagron	Griseofulvin	13L-13B08	1
Fagron	Griseofulvin	13L13-B08-290316	4
Fagron	Griseofulvin	13L13-B08-290317	1
Fagron	Griseofulvin	140410	2
Fagron	Griseofulvin	14E16-B01-300366	3
Fagron	Griseofulvin	14E16-B01-300367	1
Fagron	Griseofulvin	15062015A	1
Fagron	Griseofulvin	15810-B06	1
Fagron	Griseofulvin	15B10-B06	1
Fagron	Griseofulvin	15B10-B06-306547	9
Fagron	Griseofulvin	15B10-B06-306663	1
Fagron	Griseofulvin	15B10-B06-396547	1
Fagron	Griseofulvin	15l03-b04-315624	1
Fagron	Griseofulvin	15L03-B04-315624	3
Fagron	Griseofulvin	15L03-B315624	1
Fagron	Griseofulvin	16F13-B06	1
Fagron	Griseofulvin	16F13-B06-323067	3
Fagron	Griseofulvin	16F13-B06-323068	2
Fagron	Griseofulvin	16F13-B06-326073	1
Fagron	Griseofulvin	16f13-b06-326074	1
Fagron	Griseofulvin	16F13-B06-330832	5
Fagron	Griseofulvin	16f13-b06-330833	1
Fagron	Griseofulvin	16F13B06330833	1
Fagron	Griseofulvin	16F13-B06-330833	5
Fagron	Griseofulvin	17-L05-352461	1
Fagron	Griseofulvin	17L05-B05	5
Fagron	Griseofulvin	17L05-B05-345995	3
Fagron	Griseofulvin	17L05-B05-34999	1
Fagron	Griseofulvin	17L05-B05-351232	4
Fagron	Griseofulvin	17L05B05352461	2
Fagron	Griseofulvin	17L05-B05-352461	3
Fagron	Griseofulvin	17L05-B05-355075	1
Fagron	Griseofulvin	17LO05-B05-352461	1
Fagron	Griseofulvin	17LO5-BO5	1
Fagron	Griseofulvin	17LO5-BO5-352461	1
Fagron	Griseofulvin	17LOS-B05-351232	1
Fagron	Griseofulvin	18L04-B01	2
Fagron	Griseofulvin	18L04-B01-357660	3
Fagron	Griseofulvin	18L04-B01-357661	1
Fagron	Griseofulvin	18L04-B01-359072	2
Fagron	Griseofulvin	18L04-B01-359073	2
Fagron	Griseofulvin	18L04-B01-361614	4
Fagron	Griseofulvin	18L04-B01-361615	3
Fagron	Griseofulvin	18L04-B01-3670033	1
Fagron	Griseofulvin	18L04-BO1-357660	1
Fagron	Griseofulvin	B01-3670303	1
Fagron	Griseofulvin	HH160510	1
Fagron	Griseofulvin	HH171022	1
Fargon GmbH & Co.KG	Griseofulvin	16F13-B06-323067	1
Fargon/Sanacorp	Griseofulvin	17L05-B05-351231	1
Gehe	Griseofulvin	15B10-B06-306547	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
LAP	Griseofulvin	15L03-B04-315624	1
Noweda	Griseofulvin	16F13-B06-330833	1
Noweda	Griseofulvin	17L05-B05-345995	2
Phönix Gotha	Griseofulvin	140410	1
Sanacorp Stralsund	Griseofulvin	18L04-B01-359073	2
Sanacorp/ F	Griseofulvin	12B06-N07	1
Sanacorp	Griseofulvin	17L05-B05-345995	1

- 235 933 spectra from 1515 *Apo-Ident* customers from a total of 49 192 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Griseofulvin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Griseofulvin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	80	0	202 004
Type C	0	120	14	235 933

The substance/substance group *Griseofulvin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9007 %)	89.5522 % (> 87.3134 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20939	20939	0.00	120.54
21725	20939	14.16	122.42
23594	20939	7.81	129.71
26459	20939	10.80	129.77

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Guaifenesin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20551-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Guaifenesin; Guaifenesinum

Special notes

When selecting the *Guaifenesin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Guaifenesin	8	14	19

Second-stage model

For differentiation of the substance/substance group *Guaifenesin* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Guaifenesin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	75.64	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Guaifenesin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Guaifenesin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Guaifenesin	163333	23051	40	20161221*
Caelo	Guaifenesin	172496	23644	40	20171005*
Euro OTC	Guaifenesin	1212002-01	21287	40	20121214
Euro OTC	Guaifenesin	1506044	21864	60	20150708*
Euro OTC	Guaifenesin	1605005	22555	40	20160525*
Euro OTC	Guaifenesin	1910023	24941	40	20191114*
Euro OTC	Guaifenesin	2206012	26219	40	20220715*
Euro OTC	Guaifenesin	2206012	26219SI	20	20220715*
Fagron	Guaifenesin	22H03-B01-227258	26549	40	20220823
Fagron	Guaifenesin	22H03-B01-227258	26549SI	20	20220823

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 380 spectra of 10 reference samples from the substance/substance group *Guaifenesin*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 582 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 580 spectra of 15 reference samples from the substance/substance group *Guaifenesin*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Guaifenesin	190134	24518	40
Euro OTC	Guaifenesin	1701011	22993	40
Euro OTC	Guaifenesin	1706006	23551	40
Euro OTC	Guaifenesin	1710033	23741	40
Euro OTC	Guaifenesin	1802001	23949	40
Euro OTC	Guaifenesin	1804004	24076	40
Euro OTC	Guaifenesin	1809011	24316	40
Euro OTC	Guaifenesin	1901047	24474	40
Euro OTC	Guaifenesin	1906008	24801	40
Euro OTC	Guaifenesin	2007006	25245	40
Euro OTC	Guaifenesin	2002034	25292	40
Euro OTC	Guaifenesin	2102012	25601	40
Euro OTC	Guaifenesin	2306003	26770	40
Euro OTC	Guaifenesin	2406001	27280	40
Euro OTC	Guaifenesin	2306003	26770SI	20

- 201 504 spectra from a total of 4031 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 29 spectra from 9 *Apo-Ident* customers from 20 batches from the substance/substance group *Guaifenesin*.

- Among them are spectra of independent samples from 19 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Guaifenesin	1212002-01	1
Caelo	Guaifenesin	12277307	1
Caelo	Guaifenesin	12277311	1
Caelo	Guaifenesin	15302502	1
Caelo	Guaifenesin	15F30-b06-317816	1
Caelo	Guaifenesin	16135507	1
Caelo	Guaifenesin	1706006	1
Caelo	Guaifenesin	18018302	1
Euro OTC	Guaifenesin	1701011-01	1
Euro OTC	Guaifenesin	1706006-01	3
Euro OTC	Guaifenesin	1804004-01	1
Euro OTC	Guaifenesin	1809011-01	2
Euro OTC	Guaifenesin	18GF06347	1
Euro OTC	Guaifenesin	1906008-01	4
Euro OTC	Guaifenesin	1910023-01	1
Euro OTC	Guaifenesin	2002034-01	1
Euro OTC	Guaifenesin	2007006-01	3
Euro OTC	Guaifenesin	2102012-01	1
Euro OTC	Guaifenesin	2206012-01	1
Phoenix 05.07.2014	Guaifenesin	1402023-01	2

- 236 038 spectra from 1515 *Apo-Ident* customers from a total of 49 238 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Guaifenesin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Guaifenesin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	580	0	201 504
Type C	0	29	0	236 038

The substance/substance group *Guaifenesin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.9655 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 79.3103 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21287	21864	16.40	240.63
21864	21864	0.00	240.72
22555	22555	0.00	236.50
23051	23051	0.00	242.20
23644	23644	0.00	241.81
24941	24941	0.00	241.92
26219	26219	0.00	239.87
26549	23051	5.54	241.41

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Heparin sodium**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20638-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Heparin sodium; Heparinum natricum

Special notes

When selecting the *Heparin sodium* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Heparin sodium	7	15	30

Second-stage model

For differentiation of the substance/substance group *Heparin sodium* the following second-stage model is used:

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Heparin sodium* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	71.34	–
⋮	⋮	⋮
Sodium citrate	>50	135.15
Capsaicin	>50	277.43
Sucrose	>50	359.22
Oxybutynin hydrochloride	>50	469.38
Prednicarbate	>50	490.13
Quinine hydrochloride dihydrate	>50	553.80
Levocarnitine	>50	580.85
Pyridoxal-5-phosphate	>50	678.78
Amifampridine	>50	859.05
Ciprofloxacin hydrochloride	>50	868.17
Tetracaine	>50	926.66
Alfatradiol	>50	1031.27
Methoxsalen	>50	1037.41
Norethisterone acetate	>50	1254.84
Cyproterone acetate	>50	1356.99
Triclosan	>50	1693.44
Amitriptyline hydrochloride	>50	2474.83
Valine	>50	3559.80

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Heparin sodium* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Heparin sodium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Heparin sodium	12050009-03	21294	40	AR-15-FG-007427-02
Euro OTC	Heparin sodium	1605022-01	22804	40	9699

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Heparin sodium	12H30-N07	20798	40	1404230
Fagron	Heparin sodium	12L20-B01-317990	22824	40	20130312
Yino Pharma	Heparin sodium	YN01011170904	23978	40	20180411*
Yino Pharma	Heparin sodium	YN01011170904	23979	40	20180411*
Yino Pharma	Heparin sodium	YN01011170502	23980	40	20180411*
Yino Pharma	Heparin sodium	YN01011170502	23981	40	20180411*
Yino Pharma	Heparin sodium	YN01011170904	24195	40	20180531*
Yino Pharma	Heparin sodium	YN010182005002	25757	50	20200528*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 410 spectra of 10 reference samples from the substance/substance group *Heparin sodium*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.
- 152 552 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 750 spectra of 19 reference samples from the substance/substance group *Heparin sodium*.
- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Heparin sodium	1908030-01	25783	50
Fagron	Heparin sodium	16I26-B02-332108	23591	40
Fagron	Heparin sodium	21E10-B02-220313	26391	40
Fagron	Heparin sodium	22K21-B06-224495	26665	40
Yino Pharma	Heparin sodium	YN01011R1170803	23976	40
Yino Pharma	Heparin sodium	YN010111805002	24196	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Yino Pharma	Heparin sodium	YN010121805010	24197	40
Yino Pharma	Heparin sodium	YN01011R11901002	24907	40
Yino Pharma	Heparin sodium	YN010111906005	24908	40
Yino Pharma	Heparin sodium	YN010111906006	24909	40
Yino Pharma	Heparin sodium	YN010111907007	24910	40
Yino Pharma	Heparin sodium	YN010111908008	24911	40
Yino Pharma	Heparin sodium	YN010121810018	24912	40
Yino Pharma	Heparin sodium	YN010111910009	24984	40
Yino Pharma	Heparin sodium	YN010112107004	25758	50
Fagron	Heparin sodium	21E10-B02-220313	26391SI	20
Fagron	Heparin sodium	22K21-B06-224495	26665SI	20
Yino Pharma	Heparin sodium	YN01011R1170803	23977	40
Yino Pharma	Heparin sodium	YN01011R11901002	25756	50

- 201 334 spectra from a total of 4030 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 45 spectra from 24 *Apo-Ident* customers from 31 batches from the substance/substance group *Heparin sodium*.
- Among them are spectra of independent samples from 30 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Heparin sodium	20K06-B02-200814	1
	Heparin sodium	21E10-B02-220313	4
Caelo	Heparin sodium	16I26-B02-327885	1
Changzhou Qianhong B...	Heparin sodium	20K06-B02-200814	1
Euro OTC	Heparin sodium	1605022-02	2
Fagron	Heparin sodium	11190188SH	2
Fagron	Heparin sodium	12190453CQ	1
Fagron	Heparin sodium	12G19-B02-313422	1
Fagron	Heparin sodium	12H30-N07	2
Fagron	Heparin sodium	12120-B01-323107	1
Fagron	Heparin sodium	13G03-N13	3
Fagron	Heparin sodium	14D09-B08-293944	2
Fagron	Heparin sodium	14D09-B08-307077	1
Fagron	Heparin sodium	15A20-B02-307307	1
Fagron	Heparin sodium	16I26-B02	1
Fagron	Heparin sodium	16I26-B02-327885	1
Fagron	Heparin sodium	16I26-B02-332108	1
Fagron	Heparin sodium	16I26-B02-342640	1
Fagron	Heparin sodium	17L06-B01	1
Fagron	Heparin sodium	17L06-B01-354811	1
Fagron	Heparin sodium	18C21-B03-349501	1
Fagron	Heparin sodium	19J11B02195123	1
Fagron	Heparin sodium	20D28-B01	2
Fagron	Heparin sodium	20D28-B01-201583	2
Fagron	Heparin sodium	20K06-B02-200814	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Heparin sodium	21E10-B02-213670	2
Fagron	Heparin sodium	B01-2015803	1
Fagron	Heparin sodium	B02-1951203	1
Faron/Kehr /07.07.2020	Heparin sodium	19J11-B02-195122	1
Fiebig	Heparin sodium	16190116C0	1
Gatt-Koller	Heparin sodium	1901027	1
L31	Heparin sodium	16I26-B02-337593	1
Phoenix	Heparin sodium	5920101900	1

- 236 022 spectra from 1515 *Apo-Ident* customers from a total of 49 227 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Heparin sodium* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Heparin sodium* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	410	0	152 552
Type B	0	750	0	201 334
Type C	0	44	1	236 022

The substance/substance group *Heparin sodium* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5366 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2000 %)
Type C	100.0000 % (> 99.9007 %)	97.7778 % (> 91.1111 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20798	20798	0.00	112.89
21294	21294	0.00	76.55
22804	22804	0.00	69.95
22824	21294	19.65	99.98
23978	23978	0.00	50.38
23979	23979	0.00	51.39
23980	23980	0.00	63.70
23981	23981	0.00	76.07
24195	24195	0.00	86.76
25757	25757	0.00	93.52

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Histamine dihydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20963-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Histamine dihydrochloride; Histamini dihydrochloridum

Special notes

When selecting the *Histamine dihydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Histamine dihydrochloride	6	6	31

Second-stage model

For differentiation of the substance/substance group *Histamine dihydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Histamine dihydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Glycine	89.42	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Histamine dihydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Histamine dihydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Histamine dihydrochloride	1111004-02	20963	40	1403674
Euro OTC	Histamine dihydrochloride	1506030	21863	60	20150706*
Euro OTC	Histamine dihydrochloride	2004012	25166	40	20200525*
Euro OTC	Histamine dihydrochloride	2009009	25413	40	20201005*
Fagron	Histamine dihydrochloride	14G16-B02-299175	21668	100	20140729
Fagron	Histamine dihydrochloride	19D19-B02-361228	24589	40	20190516

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 320 spectra of 6 reference samples from the substance/substance group *Histamine dihydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 340 spectra of 10 reference samples from the substance/substance group *Histamine dihydrochloride*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Histamine dihydrochloride	1812018	24541	40
Euro OTC	Histamine dihydrochloride	1905003	24616	40
Euro OTC	Histamine dihydrochloride	2301007	26526	40
Euro OTC	Histamine dihydrochloride	2409007	27453	40
Fagron	Histamine dihydrochloride	15C25-B50-331242	23196	40
Fagron	Histamine dihydrochloride	22H25-B01-222394	26389	40
Euro OTC	Histamine dihydrochloride	2301007	26526SI	20
Euro OTC	Histamine dihydrochloride	2409007	27453SI	20
Fagron	Histamine dihydrochloride	15C25-B50-331242	23197	40
Fagron	Histamine dihydrochloride	22H25-B01-222394	26389SI	20

- 201 744 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 61 spectra from 32 *Apo-Ident* customers from 34 batches from the substance/substance group *Histamine dihydrochloride*.

- Among them are spectra of independent samples from 31 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Histamine dihydrochloride	1111004-02	1
Caelo	Histamine dihydrochloride	130500601	1
Euro OTC	Histamine dihydrochloride	1104004-03	1
Euro OTC	Histamine dihydrochloride	111004-02	1
Euro OTC	Histamine dihydrochloride	1111004-01	5
Euro OTC	Histamine dihydrochloride	1111004-02	1
Euro OTC	Histamine dihydrochloride	12K06-N08	2
Euro OTC	Histamine dihydrochloride	1305006-01	1
Euro OTC	Histamine dihydrochloride	1411012-02	4
Euro OTC	Histamine dihydrochloride	1411012-03	1
Euro OTC	Histamine dihydrochloride	1506030-01	3
Euro OTC	Histamine dihydrochloride	1811014-01	1
Euro OTC	Histamine dihydrochloride	1812018-01	1
Euro OTC	Histamine dihydrochloride	1905003-01	2
Euro OTC	Histamine dihydrochloride	1905003-02	3
Euro OTC	Histamine dihydrochloride	20021412	1
Euro OTC	Histamine dihydrochloride	2004012-01	1
Euro OTC	Histamine dihydrochloride	3031503	1
Fa Roth	Histamine dihydrochloride	47252901	1
Fagron	Histamine dihydrochloride	11E25-N07	2
Fagron	Histamine dihydrochloride	12D02-N16	1
Fagron	Histamine dihydrochloride	12E29-N09	3
Fagron	Histamine dihydrochloride	12K06-N08	5
Fagron	Histamine dihydrochloride	1305006-01	1
Fagron	Histamine dihydrochloride	14J06B01299179	1
Fagron	Histamine dihydrochloride	15E08-B06-313037	3
Fagron	Histamine dihydrochloride	17D11-B001-339451	1
Fagron	Histamine dihydrochloride	19D19-B02-361228	1
Fagron	Histamine dihydrochloride	28051305	1
Fagron	Histamine dihydrochloride	454545	1
Fagron	Histamine dihydrochloride	L17100130-OF-222030	1
Fargon/Fargon	Histamine dihydrochloride	19019-B02	1
Fargon/Fargon	Histamine dihydrochloride	19D19-B02	1
Fargon/Fargon	Histamine dihydrochloride	19H23-F04-364053	3
Merck	Histamine dihydrochloride	Wxbc3407V	1
Merck	Histamine dihydrochloride	WXBC3407V	1
Sanacop	Histamine dihydrochloride	15C25-B01-306047	1

- 236 006 spectra from 1515 *Apo-Ident* customers from a total of 49 225 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Histamine dihydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Histamine dihydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	340	0	201 744
Type C	0	61	0	236 006

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The substance/substance group *Histamine dihydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.2353 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 90.1639 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20963	20963	0.00	154.87
21668	21863	11.73	158.77
21863	21863	0.00	155.50
24589	25166	6.94	154.49
25166	25166	0.00	154.59
25413	25413	0.00	152.70

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Histidine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	23135-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Histidine; Histidinum; L-histidine

Special notes

When selecting the *Histidine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Histidine	6	4	1

Second-stage model

For differentiation of the substance/substance group *Histidine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Histidine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Glycine	115.89	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Histidine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Histidine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Histidine	1703022	23135	40	20170405*
Euro OTC	Histidine	2004038	25163	40	20200528*
Euro OTC	Histidine	2101009	25577	40	20210121*
Euro OTC	Histidine	2301009	26520	40	20230201*
Euro OTC	Histidine	2301009	26520SI	20	20230201*
Fagron	Histidine	15I01-B12-329082	23590	40	20150921
Fagron	Histidine	18J03-B02-355093	24701	40	20181123

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 260 spectra of 7 reference samples from the substance/substance group *Histidine*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 6 reference samples from the substance/substance group *Histidine*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Histidine	2201021	25953	40
Fagron	Histidine	17F15-B04-343276	23935	40
Fagron	Histidine	20J15-B01-202794	25487	40
Fagron	Histidine	23C07-B06-229457	26684	40
Euro OTC	Histidine	2201021	25953SI	10
Fagron	Histidine	23C07-B06-229457	26684SI	20

- 201 894 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Histidine*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Histidine	2004038-01	1

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Histidine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Histidine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	190	0	201 894
Type C	0	1	0	236 066

The substance/substance group *Histidine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23135	23135	0.00	186.79
23590	25577	5.53	187.73
24701	25577	4.86	187.79
25163	25163	0.00	186.70
25577	25577	0.00	186.89
26520	26520	0.00	188.12

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Homatropine hydrobromide**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	24442-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Homatropine hydrobromide; Homatropini hydrobromidum

Special notes

When selecting the *Homatropine hydrobromide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Homatropine hydrobromide	2	2	0

Second-stage model

For differentiation of the substance/substance group *Homatropine hydrobromide* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Homatropine hydrobromide* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	120.04	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Homatropine hydrobromide* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Homatropine hydrobromide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Homatropine hydrobromide	18L11-B03-356938	24442	40	1905511
Fagron	Homatropine hydrobromide	23G12-B16-233048	27020	40	20230726
Fagron	Homatropine hydrobromide	23G12-B16-233048	27020SI	20	20230726

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 100 spectra of 3 reference samples from the substance/substance group *Homatropine hydrobromide*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 862 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 4 reference samples from the substance/substance group *Homatropine hydrobromide*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Homatropine hydrobromide	21J07-B04-213599	26056	40
Fagron	Homatropine hydrobromide	24D24-B09-000930	27375	40
Fagron	Homatropine hydrobromide	21J07-B04-213599	26056SI	20
Fagron	Homatropine hydrobromide	24D24-B09-000930	27375SI	20

- 201 964 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Homatropine hydrobromide*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Homatropine hydrobromide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Homatropine hydrobromide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	100	0	152 862
Type B	0	120	0	201 964
Type C	0	0	0	236 067

The substance/substance group *Homatropine hydrobromide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24442	24442	0.00	185.05
27020	24442	7.75	182.27

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hydrochlorothiazide**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20323-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hydrochlorothiazide; Hydrochlorothiazidum

Special notes

When selecting the *Hydrochlorothiazide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hydrochlorothiazide	6	4	111

Second-stage model

For differentiation of the substance/substance group *Hydrochlorothiazide* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hydrochlorothiazide* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	113.22	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hydrochlorothiazide* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hydrochlorothiazide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hydrochlorothiazide	13008505	21589	60	AR-15-FG-014461-01
Caelo	Hydrochlorothiazide	182649	24362	40	20181127*
Fagron	Hydrochlorothiazide	11L01-N02	20888	40	20111209
Fagron	Hydrochlorothiazide	17L20-B02-345079	23989	40	20180125
Fagron	Hydrochlorothiazide	20E27-F01-371506	25590	40	20200630
Fagron	Hydrochlorothiazide	21H27-B04-220130	26172	40	20220202

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 6 reference samples from the substance/substance group *Hydrochlorothiazide*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 6 reference samples from the substance/substance group *Hydrochlorothiazide*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydrochlorothiazide	14009701	23116	40
Caelo	Hydrochlorothiazide	192328	24888	40
Caelo	Hydrochlorothiazide	23002418	27125	40
Fagron	Hydrochlorothiazide	16F17-B07-327489	23600	40
Caelo	Hydrochlorothiazide	23002418	27125SI	20
Fagron	Hydrochlorothiazide	21H27-B04-220130	26172SI†	20

- 201 884 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 440 spectra from 264 *Apo-Ident* customers from 120 batches from the substance/substance group *Hydrochlorothiazide*.
- Among them are spectra of independent samples from 110 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Hydrochlorothiazide	18017305	1
	Hydrochlorothiazide	20004000011	1
	Hydrochlorothiazide	20004000014	1
	Hydrochlorothiazide	22044HC10RII	1
	Hydrochlorothiazide	22K29-B01-224324	3
	Hydrochlorothiazide	23002418002	1
	Hydrochlorothiazide	23A04-B06-229298	3
	Hydrochlorothiazide	23L28-B02-237422	1
	Hydrochlorothiazide	B06-2336203	1
AHD	Hydrochlorothiazide	17H28-B01-340561	1
Caelo	Hydrochlorothiazide	11101n02	1
Caelo	Hydrochlorothiazide	13008507	2
Caelo	Hydrochlorothiazide	13008509	5
Caelo	Hydrochlorothiazide	14009701	25
Caelo	Hydrochlorothiazide	140097012	1
Caelo	Hydrochlorothiazide	14B10-B01-294558	2
Caelo	Hydrochlorothiazide	14B10-B01-305043	2
Caelo	Hydrochlorothiazide	15231002	3
Caelo	Hydrochlorothiazide	15231003	5
Caelo	Hydrochlorothiazide	15231005	1
Caelo	Hydrochlorothiazide	15231008	2
Caelo	Hydrochlorothiazide	15231009	3
Caelo	Hydrochlorothiazide	15231011	1
Caelo	Hydrochlorothiazide	16269301	4
Caelo	Hydrochlorothiazide	16269304	2
Caelo	Hydrochlorothiazide	16269306	1
Caelo	Hydrochlorothiazide	16269307	3
Caelo	Hydrochlorothiazide	16269309	6
Caelo	Hydrochlorothiazide	16269311	3
Caelo	Hydrochlorothiazide	16269312	2
Caelo	Hydrochlorothiazide	16269313	4
Caelo	Hydrochlorothiazide	16F17-B07-324062	1
Caelo	Hydrochlorothiazide	16F17B07327489	1
Caelo	Hydrochlorothiazide	16F17-B07-327489	1
Caelo	Hydrochlorothiazide	17H28-B01-340561	1
Caelo	Hydrochlorothiazide	17L20-B02-345079	1
Caelo	Hydrochlorothiazide	18017301	2
Caelo	Hydrochlorothiazide	18017302	5
Caelo	Hydrochlorothiazide	18017303	1
Caelo	Hydrochlorothiazide	18017304	6
Caelo	Hydrochlorothiazide	18017305	10
Caelo	Hydrochlorothiazide	18017307	3
Caelo	Hydrochlorothiazide	18108HCRII	1
Caelo	Hydrochlorothiazide	182649005	1
Caelo	Hydrochlorothiazide	18264901	7
Caelo	Hydrochlorothiazide	18264904	7
Caelo	Hydrochlorothiazide	18264907	6
Caelo	Hydrochlorothiazide	1923280002	1
Caelo	Hydrochlorothiazide	192328002	14
Caelo	Hydrochlorothiazide	20004000002	9
Caelo	Hydrochlorothiazide	20004000004	4
Caelo	Hydrochlorothiazide	20004000007	2
Caelo	Hydrochlorothiazide	20004000010	3
Caelo	Hydrochlorothiazide	20004000011	2
Caelo	Hydrochlorothiazide	2000400002	1
Caelo	Hydrochlorothiazide	2000400004	1
Caelo	Hydrochlorothiazide	2004000002	1
Caelo	Hydrochlorothiazide	20E27-F01-371506	1
Caelo	Hydrochlorothiazide	F01-3715006	1
Caeol/ Noweda	Hydrochlorothiazide	15231009	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Hydrochlorothiazide	18264907	2
Caesar & Loretz GmbH...	Hydrochlorothiazide	192328002	1
Caesar & Loretz GmbH...	Hydrochlorothiazide	20004000007	1
Caesar & Loretz GmbH...	Hydrochlorothiazide	20004000004	1
Caesar & Loretz GmbH/Gehe	Hydrochlorothiazide	18017304	1
Caesar & Loretz GmbH/Gehe	Hydrochlorothiazide	18264904	1
Caesar & Loretz GmbH/Gehe	Hydrochlorothiazide	18264906	1
Caesar & Loretz GmbH/Gehe	Hydrochlorothiazide	18264907	1
Caesar & Loretz GmbH...	Hydrochlorothiazide	18017307	1
Caesar & Loretz GmbH	Hydrochlorothiazide	18017305	3
Caesar & Loretz GmbH	Hydrochlorothiazide	18017307	1
Caesar & Loretz GmbH	Hydrochlorothiazide	18264901	1
Caesar & Loretz GmbH	Hydrochlorothiazide	18264904	4
Caesar & Loretz GmbH	Hydrochlorothiazide	18264907	1
Caesar & Loretz GmbH	Hydrochlorothiazide	192328002	14
Caesar & Loretz GmbH	Hydrochlorothiazide	20004000002	5
Caesar & Loretz GmbH	Hydrochlorothiazide	20004000003	1
Caesar & Loretz GmbH	Hydrochlorothiazide	20004000004	1
Caesar & Loretz GmbH	Hydrochlorothiazide	20004000007	4
Caesar & Loretz GmbH	Hydrochlorothiazide	20004000010	1
Caesar & Loretz GmbH	Hydrochlorothiazide	20004000011	1
Caesar & Loretz	Hydrochlorothiazide	18017302	1
Fagron	Hydrochlorothiazide		1
Fagron	Hydrochlorothiazide	11E04-N10	1
Fagron	Hydrochlorothiazide	11G12-N12	1
Fagron	Hydrochlorothiazide	11l01-n02	2
Fagron	Hydrochlorothiazide	11L01-N02	2
Fagron	Hydrochlorothiazide	11L01-No2	1
Fagron	Hydrochlorothiazide	11Lo1-No2	1
Fagron	Hydrochlorothiazide	12A03-B40	3
Fagron	Hydrochlorothiazide	12A03-B40-286110	1
Fagron	Hydrochlorothiazide	12A03-B40-286111	3
Fagron	Hydrochlorothiazide	12E04-N02	1
Fagron	Hydrochlorothiazide	12L14-N11	4
Fagron	Hydrochlorothiazide	13008504	1
Fagron	Hydrochlorothiazide	13C25-N08	6
Fagron	Hydrochlorothiazide	14B10B01	1
Fagron	Hydrochlorothiazide	14B10-B01	2
Fagron	Hydrochlorothiazide	14b10-b01-294558	1
Fagron	Hydrochlorothiazide	14B10-B01-294558	4
Fagron	Hydrochlorothiazide	14B10-B01-300822	2
Fagron	Hydrochlorothiazide	14B10-B01-305043	3
Fagron	Hydrochlorothiazide	15E04-B03	1
Fagron	Hydrochlorothiazide	15E04-B03-309670	5
Fagron	Hydrochlorothiazide	15K16	1
Fagron	Hydrochlorothiazide	15K16-B01	4
Fagron	Hydrochlorothiazide	15K16-B01-315836	3
Fagron	Hydrochlorothiazide	15K16-B01-319833	9
Fagron	Hydrochlorothiazide	16F17-B07	2
Fagron	Hydrochlorothiazide	16F17-B07-322773	1
Fagron	Hydrochlorothiazide	16F17-B07-324062	5
Fagron	Hydrochlorothiazide	16F17-B07-327489	5
Fagron	Hydrochlorothiazide	17038HCRII	1
Fagron	Hydrochlorothiazide	17H28-B01340561	1
Fagron	Hydrochlorothiazide	17H28-B01-340561	4
Fagron	Hydrochlorothiazide	17L20-B02	1
Fagron	Hydrochlorothiazide	17L20-B02-345079	5
Fagron	Hydrochlorothiazide	17L20-B02-347789	6
Fagron	Hydrochlorothiazide	17L20-B02-349593	6
Fagron	Hydrochlorothiazide	17L20-B02-353429	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Hydrochlorothiazide	17L20B02355636	1
Fagron	Hydrochlorothiazide	17L20-B02-355636	6
Fagron	Hydrochlorothiazide	17L20B05	1
Fagron	Hydrochlorothiazide	19100HCRII	1
Fagron	Hydrochlorothiazide	19A04-B01	4
Fagron	Hydrochlorothiazide	19A04-B01-359105	5
Fagron	Hydrochlorothiazide	19a04-b01-363321	1
Fagron	Hydrochlorothiazide	19A04-B01-363321	7
Fagron	Hydrochlorothiazide	2002311234	1
Fagron	Hydrochlorothiazide	20E27-F01	4
Fagron	Hydrochlorothiazide	20E27-F01-371506	10
Fagron	Hydrochlorothiazide	20E27-F01-373727	4
Fagron	Hydrochlorothiazide	21H27-B04-216272	5
Fagron	Hydrochlorothiazide	21H27-B04-220130	3
Fagron	Hydrochlorothiazide	22K29-B01-224324	3
Fagron	Hydrochlorothiazide	27101804	1
Fagron	Hydrochlorothiazide	5013Q-03660	1
Fagron	Hydrochlorothiazide	B04-2162702	1
Fagron	Hydrochlorothiazide	C01-20150412	1
Fagron	Hydrochlorothiazide	c01-20160510	1
Fagron	Hydrochlorothiazide	C01-20160510	1
Fagron	Hydrochlorothiazide	Co1-20150412	1
Fagron	Hydrochlorothiazide	CQ1108	1
Fagron	Hydrochlorothiazide	CR0601	1
Fagron	Hydrochlorothiazide	F01-3737207	1
Fargon - Alliance He...	Hydrochlorothiazide	17L20-B02-353429	1
Fargon/Phönix	Hydrochlorothiazide	16F17-B07-327489	1
Fiebig	Hydrochlorothiazide	115231003	1
Fiebig	Hydrochlorothiazide	19100hcrII	1
Fiebig	Hydrochlorothiazide	B01-3633201	1
Gehe	Hydrochlorothiazide	12E04-N02	1
Gehe	Hydrochlorothiazide	17L20-B02-353429	1
Gehe	Hydrochlorothiazide	17L20-B02-355636	1
GEHE	Hydrochlorothiazide	18017302	1
Gehe	Hydrochlorothiazide	18017304	1
Gehe	Hydrochlorothiazide	23002418002	1
Kehr	Hydrochlorothiazide	20004000011	1
Kehr	Hydrochlorothiazide	23A04-B06-229298	1
noweda	Hydrochlorothiazide	15231009	1
Noweda	Hydrochlorothiazide	16269307	1
Noweda	Hydrochlorothiazide	23A04-B06-229298	2
Phoenix	Hydrochlorothiazide	15231003	1
Phoenix	Hydrochlorothiazide	17L20-B02-347789	1
Phoenix	Hydrochlorothiazide	18017302	2
Phoenix	Hydrochlorothiazide	18264901	1
Phoenix	Hydrochlorothiazide	18264904	2
Phönix	Hydrochlorothiazide	192328002	1
Sanacorp	Hydrochlorothiazide	12A03-B40-26111	1
Sanacorp	Hydrochlorothiazide	15231008	1
Sanacorp	Hydrochlorothiazide	16269302	1
Sanacorp	Hydrochlorothiazide	18017302	1
Sanacorp	Hydrochlorothiazide	19A04-B01	2
Sanacorp	Hydrochlorothiazide	22K29-B01-224324	1
Sanacorp	Hydrochlorothiazide	23A04-B06-233623	1

- 235 627 spectra from 1515 *Apo-Ident* customers from a total of 49 138 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hydrochlorothiazide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hydrochlorothiazide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	200	0	201 884
Type C	0	430	10	235 627

The substance/substance group *Hydrochlorothiazide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9007 %)	97.7273 % (> 97.0455 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20888	21589	16.49	313.30
21589	21589	0.00	318.78
23989	24362	5.89	323.75
24362	24362	0.00	324.85
25590	24362	5.39	322.87
26172	24362	9.40	322.94

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hydrocortisone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20006-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hydrocortisone; Hydrocortisonum

Special notes

When selecting the *Hydrocortisone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hydrocortisone	9	11	544

Second-stage model

For differentiation of the substance/substance group *Hydrocortisone* the following second-stage model is used:

- Submodel 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hydrocortisone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	83.00	–
⋮	⋮	⋮
Mometasone furoate	>50	117.19
Escin, water-soluble	>50	157.42
Potassium sorbate	>50	170.67
Magnesium hydrogen citrate	>50	180.36
Atropine sulfate	>50	221.65
Quinoline yellow	>50	373.09
Calcium orotate dihydrate	>50	487.26
Propranolol hydrochloride	>50	571.76
Saccharin sodium	>50	609.19
Phenytoin	>50	850.49

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hydrocortisone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hydrocortisone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hydrocortisone	13341502	21461	60	20131203
Caelo	Hydrocortisone	13341502	21463	60	20131203
Caelo	Hydrocortisone	180915	24020	40	20180412*
Euro OTC	Hydrocortisone	1206018-01	21293	40	20130727
Euro OTC	Hydrocortisone	1509029	21899	60	20151014*
Euro OTC	Hydrocortisone	1509029	21899SI	51	20151014*
Euro OTC	Hydrocortisone	1611016	22910	40	20161220*
Euro OTC	Hydrocortisone	2101003	25571	40	20210128*
Euro OTC	Hydrocortisone	2101003	25571SI	40	20210128*
Fagron	Hydrocortisone	16A19-B06-320970	22829	40	20160204

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Hydrocortisone	16A19-B06-320970	22829SI	30	20160204
Fagron	Hydrocortisone	16A19-B06-321981	22837	40	20160204
Fagron	Hydrocortisone	16A19-B06-321981	22838	40	1702302
Fagron	Hydrocortisone	16H01-B01-326071	22928	40	20160907
Fagron	Hydrocortisone	16H01-B01-326071	22928SI	40	20160907

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 661 spectra of 15 reference samples from the substance/substance group *Hydrocortisone*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 301 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1119 spectra of 29 reference samples from the substance/substance group *Hydrocortisone*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydrocortisone	160952	22778	40
Caelo	Hydrocortisone	171194	23340	20
Caelo	Hydrocortisone	172566	23840	40
Caelo	Hydrocortisone	183243	24521	40
Caelo	Hydrocortisone	21001215005	25926	40
Caelo	Hydrocortisone	22003779	27250	40
Euro OTC	Hydrocortisone	1802009	23945	40
Euro OTC	Hydrocortisone	1906033	24771	40
Euro OTC	Hydrocortisone	2205003	26213	40
Euro OTC	Hydrocortisone	2401017	27152	40
Fagron	Hydrocortisone	22E09-B02-220942	26395	40

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydrocortisone	13341502	21463SI†	60
Caelo	Hydrocortisone	160952	22778SI	40
Caelo	Hydrocortisone	171194	23340SI	28
Caelo	Hydrocortisone	171194	23659	40
Caelo	Hydrocortisone	171194	23659SI	30
Caelo	Hydrocortisone	172566	23840SI	40
Caelo	Hydrocortisone	180915	24020SI†	40
Caelo	Hydrocortisone	183243	24521SI	40
Caelo	Hydrocortisone	21001215005	25926SI	40
Caelo	Hydrocortisone	22003779	27250SI	40
Euro OTC	Hydrocortisone	1611016	22910SI†	40
Euro OTC	Hydrocortisone	1802009	23945SI	40
Euro OTC	Hydrocortisone	1906033	24771SI	40
Euro OTC	Hydrocortisone	2205003	26213SI	40
Euro OTC	Hydrocortisone	2401017	27152SI	40
Fagron	Hydrocortisone	16A19-B06-321981	22837SI†	30
Fagron	Hydrocortisone	16A19-B06-321981	22838SI†	31
Fagron	Hydrocortisone	22E09-B02-220942	26395SI	40

- 200 965 spectra from a total of 4030 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4496 spectra from 1108 *Apo-Ident* customers from 564 batches from the substance/substance group *Hydrocortisone*.
- Among them are spectra of independent samples from 544 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Hydrocortisone	2100121029	1
	Hydrocortisone	21001215017	2
	Hydrocortisone	21001215018	2
	Hydrocortisone	21001215019	2
	Hydrocortisone	21001215023	3
	Hydrocortisone	21001215026	2
	Hydrocortisone	21001215027	3
	Hydrocortisone	21001215029	7
	Hydrocortisone	21001215030	7
	Hydrocortisone	21001215032	3
	Hydrocortisone	21001215034	10
	Hydrocortisone	21001215035	3
	Hydrocortisone	21001215036	4
	Hydrocortisone	2200377900	1
	Hydrocortisone	22003779003	2
	Hydrocortisone	22003779004	17

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Hydrocortisone	22003779005	4
	Hydrocortisone	22003779006	18
	Hydrocortisone	22003779008	2
	Hydrocortisone	22003779011	1
	Hydrocortisone	22003779012	3
	Hydrocortisone	220500301	1
	Hydrocortisone	2205003-01	8
	Hydrocortisone	22E09-B02-219558	1
	Hydrocortisone	23003407002	1
	Hydrocortisone	23D06-B01-232991	1
	Hydrocortisone	K05M20211103	1
/ AHD	Hydrocortisone	16095202	1
A.H. 10.06.13 ek: 10,01EUR	Hydrocortisone	1204037-01	1
AEP	Hydrocortisone	21001215015	1
AEP	Hydrocortisone	21001215032	1
AHC 02.09.13 EK9,85	Hydrocortisone	1112030-01	1
AHC	Hydrocortisone	22003779006	1
ahd,11,95EUR 10.04.14	Hydrocortisone	13341504-07R07	1
AHD/Euro	Hydrocortisone	1802009	1
AHD/Euro	Hydrocortisone	1802009-01	2
AHD	Hydrocortisone	13069507	1
AHD	Hydrocortisone	18091503	1
AHD	Hydrocortisone	18091520	1
AHD	Hydrocortisone	21001215021	2
AHD	Hydrocortisone	21001215032	1
AHD	Hydrocortisone	22003779004	1
AHD	Hydrocortisone	22003779011	2
AHD	Hydrocortisone	2205003-01	1
AHD;19.06.15;18,70EUR	Hydrocortisone	14301306	1
AHL	Hydrocortisone	15125-B01-313084	1
Alliance Healtcare	Hydrocortisone	192241008	1
Alliance Healtcare	Hydrocortisone	21001215018	1
Alliance Health 11.0...	Hydrocortisone	1315505	1
Alliance Health25.04.2014	Hydrocortisone	13341503	3
Alliance Healthcare	Hydrocortisone	192241005	1
Alliance	Hydrocortisone	21001215021	1
Allianz Healthcare	Hydrocortisone	1509029-01	1
Allianz Healthcare	Hydrocortisone	1802009-01	1
Anzag 14.12.12 ek:10,01	Hydrocortisone	1202032-01	1
Anzag ek:10.01EUR 18.07.12	Hydrocortisone	1107005-03	1
Anzag	Hydrocortisone	1107005-02	1
Anzag	Hydrocortisone	11260305	1
Anzag	Hydrocortisone	1206018-01	1
Anzag	Hydrocortisone	12104307	1
Anzag	Hydrocortisone	14301306	1
Anzag	Hydrocortisone	1501034-01	1
Anzag	Hydrocortisone	1505016-01	1
Anzag	Hydrocortisone	1509229-01	1
Anzag	Hydrocortisone	183243006	1
Anzag	Hydrocortisone	192241007	1
Anzag	Hydrocortisone	19224107	1
Anzag	Hydrocortisone	20004116003	2
Anzag	Hydrocortisone	20004116007	1
Anzag	Hydrocortisone	21001215019	1
Beiersdorf/ Vedono	Hydrocortisone	15181004	1
Berkel AHK	Hydrocortisone	14301305	1
Bionorica	Hydrocortisone	16004604	1
Bombastus	Hydrocortisone	14I05-B02-300227	1
cae	Hydrocortisone	18324307	1
Caeelo	Hydrocortisone	17090005	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
cael	Hydrocortisone	183243002	1
Caelo	Hydrocortisone		2
Caelo	Hydrocortisone	10071704	1
Caelo	Hydrocortisone	10282208	1
Caelo	Hydrocortisone	11021302	1
Caelo	Hydrocortisone	1109845	1
Caelo	Hydrocortisone	11260308	3
Caelo	Hydrocortisone	11260309	3
Caelo	Hydrocortisone	11273704	1
Caelo	Hydrocortisone	113I-01719	1
Caelo	Hydrocortisone	1140317	1
Caelo	Hydrocortisone	1190218/17256602	1
Caelo	Hydrocortisone	120403701	1
Caelo	Hydrocortisone	12104301	1
Caelo	Hydrocortisone	12104303	5
Caelo	Hydrocortisone	12104304	6
Caelo	Hydrocortisone	12104305	3
Caelo	Hydrocortisone	12104306	9
Caelo	Hydrocortisone	12104307	17
Caelo	Hydrocortisone	12104308	8
Caelo	Hydrocortisone	12104309	2
Caelo	Hydrocortisone	12119303	8
Caelo	Hydrocortisone	12119304	4
Caelo	Hydrocortisone	12167001	7
Caelo	Hydrocortisone	12167007	10
Caelo	Hydrocortisone	12167010	10
Caelo	Hydrocortisone	12167010-3437311151	1
Caelo	Hydrocortisone	1216707	1
Caelo	Hydrocortisone	12k08-n01	1
Caelo	Hydrocortisone	130617H	1
Caelo	Hydrocortisone	13063501	1
Caelo	Hydrocortisone	1306906	1
Caelo	Hydrocortisone	13069501	10
Caelo	Hydrocortisone	13069502	5
Caelo	Hydrocortisone	13069505	4
Caelo	Hydrocortisone	13069506	8
Caelo	Hydrocortisone	13069507	4
Caelo	Hydrocortisone	13069509	2
Caelo	Hydrocortisone	13069510	6
Caelo	Hydrocortisone	13155601	9
Caelo	Hydrocortisone	13155602	8
Caelo	Hydrocortisone	13155603	12
Caelo	Hydrocortisone	13155604	8
Caelo	Hydrocortisone	13155605	3
Caelo	Hydrocortisone	13155611	2
Caelo	Hydrocortisone	13155614	3
Caelo	Hydrocortisone	133341502	1
Caelo	Hydrocortisone	13341501	7
Caelo	Hydrocortisone	13341502	11
Caelo	Hydrocortisone	13341503	1
Caelo	Hydrocortisone	13341504	7
Caelo	Hydrocortisone	13341508	4
Caelo	Hydrocortisone	13341509	8
Caelo	Hydrocortisone	13341510	12
Caelo	Hydrocortisone	13341511	5
Caelo	Hydrocortisone	13342504	1
Caelo	Hydrocortisone	140301305	1
Caelo	Hydrocortisone	14115103	2
Caelo	Hydrocortisone	14115104	1
Caelo	Hydrocortisone	14115105	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hydrocortisone	14115107	11
Caelo	Hydrocortisone	14115108	2
Caelo	Hydrocortisone	14301304	4
Caelo	Hydrocortisone	14301305	5
Caelo	Hydrocortisone	14301306	6
Caelo	Hydrocortisone	14301307	2
Caelo	Hydrocortisone	14301310	14
Caelo	Hydrocortisone	14301311	10
Caelo	Hydrocortisone	14301312	8
Caelo	Hydrocortisone	14301313	6
Caelo	Hydrocortisone	14b04-B02-293422	1
Caelo	Hydrocortisone	15/25-B01-318486	1
Caelo	Hydrocortisone	1501034-01	2
Caelo	Hydrocortisone	15021104	7
Caelo	Hydrocortisone	15021105	7
Caelo	Hydrocortisone	15021106	3
Caelo	Hydrocortisone	15021107	11
Caelo	Hydrocortisone	1505016-01	3
Caelo	Hydrocortisone	1509029-01	5
Caelo	Hydrocortisone	1518012	1
Caelo	Hydrocortisone	1518013	1
Caelo	Hydrocortisone	15181003	11
Caelo	Hydrocortisone	15181004	11
Caelo	Hydrocortisone	15181006	20
Caelo	Hydrocortisone	15181007	5
Caelo	Hydrocortisone	15181008	2
Caelo	Hydrocortisone	15181012	16
Caelo	Hydrocortisone	15181012/20160309/10	1
Caelo	Hydrocortisone	15181013	11
Caelo	Hydrocortisone	15181014	6
Caelo	Hydrocortisone	15216101	10
Caelo	Hydrocortisone	15278702	11
Caelo	Hydrocortisone	15278703	9
Caelo	Hydrocortisone	15278705	11
Caelo	Hydrocortisone	15278706	6
Caelo	Hydrocortisone	16004603	14
Caelo	Hydrocortisone	16004604	28
Caelo	Hydrocortisone	16004605	14
Caelo	Hydrocortisone	16004607	16
Caelo	Hydrocortisone	16004608	12
Caelo	Hydrocortisone	16004611	11
Caelo	Hydrocortisone	16004612	16
Caelo	Hydrocortisone	16004612/2020317	1
Caelo	Hydrocortisone	16041801	1
Caelo	Hydrocortisone	16095201	27
Caelo	Hydrocortisone	16095202	12
Caelo	Hydrocortisone	16095203	10
Caelo	Hydrocortisone	16095207	8
Caelo	Hydrocortisone	16095209	7
Caelo	Hydrocortisone	16095210	24
Caelo	Hydrocortisone	16095212	8
Caelo	Hydrocortisone	16095213	13
Caelo	Hydrocortisone	16095213-20170704Ma7	1
Caelo	Hydrocortisone	16098201	2
Caelo	Hydrocortisone	1611016	1
Caelo	Hydrocortisone	1611016-01	5
Caelo	Hydrocortisone	16255603	10
Caelo	Hydrocortisone	16255604	2
Caelo	Hydrocortisone	16255606	1
Caelo	Hydrocortisone	16255607	13

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hydrocortisone	16255608	15
Caelo	Hydrocortisone	16255608NP	1
Caelo	Hydrocortisone	16255680	1
Caelo	Hydrocortisone	1626-B04-330340	1
Caelo	Hydrocortisone	16272304	13
Caelo	Hydrocortisone	16272305	11
Caelo	Hydrocortisone	16272306	14
Caelo	Hydrocortisone	16272308	5
Caelo	Hydrocortisone	1627231	1
Caelo	Hydrocortisone	16272311	7
Caelo	Hydrocortisone	1672305	1
Caelo	Hydrocortisone	1672308	1
Caelo	Hydrocortisone	167272306	1
Caelo	Hydrocortisone	17090003	4
Caelo	Hydrocortisone	17090004	1
Caelo	Hydrocortisone	17090005	8
Caelo	Hydrocortisone	170921HA/17090003	1
Caelo	Hydrocortisone	1711940	1
Caelo	Hydrocortisone	17119402	21
Caelo	Hydrocortisone	17119403	24
Caelo	Hydrocortisone	17119404	1
Caelo	Hydrocortisone	17119405	36
Caelo	Hydrocortisone	17119406	23
Caelo	Hydrocortisone	17119407	31
Caelo	Hydrocortisone	17119410	7
Caelo	Hydrocortisone	1719402-20171106Ma2	1
Caelo	Hydrocortisone	1719405	1
Caelo	Hydrocortisone	17229410	1
Caelo	Hydrocortisone	17256602	56
Caelo	Hydrocortisone	17256603	10
Caelo	Hydrocortisone	17256604	36
Caelo	Hydrocortisone	17256605	26
Caelo	Hydrocortisone	17256607	15
Caelo	Hydrocortisone	17256804	1
Caelo	Hydrocortisone	1726602	1
Caelo	Hydrocortisone	1726603	1
Caelo	Hydrocortisone	1731205	1
Caelo	Hydrocortisone	173512	1
Caelo	Hydrocortisone	173512005	1
Caelo	Hydrocortisone	17351202	19
Caelo	Hydrocortisone	17351203	36
Caelo	Hydrocortisone	17351205	65
Caelo	Hydrocortisone	17351206	11
Caelo	Hydrocortisone	17351209	11
Caelo	Hydrocortisone	17351209-20180830Ma3	1
Caelo	Hydrocortisone	17351210	2
Caelo	Hydrocortisone	1735123	1
Caelo	Hydrocortisone	17526602	1
Caelo	Hydrocortisone	1756602	1
Caelo	Hydrocortisone	17E10-B04-334857	1
Caelo	Hydrocortisone	18002009-01	1
Caelo	Hydrocortisone	1802009-01	3
Caelo	Hydrocortisone	1802009-1	2
Caelo	Hydrocortisone	18031508	1
Caelo	Hydrocortisone	18042601	1
Caelo	Hydrocortisone	18061802	1
Caelo	Hydrocortisone	18062003	1
Caelo	Hydrocortisone	18091501	27
Caelo	Hydrocortisone	18091501-H20181115Ma	3
Caelo	Hydrocortisone	18091502	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hydrocortisone	18091503	36
Caelo	Hydrocortisone	18091505	38
Caelo	Hydrocortisone	18091506	30
Caelo	Hydrocortisone	18091507	33
Caelo	Hydrocortisone	18091508	8
Caelo	Hydrocortisone	18091519	41
Caelo	Hydrocortisone	18091520	36
Caelo	Hydrocortisone	180915208	1
Caelo	Hydrocortisone	18091521	2
Caelo	Hydrocortisone	18091524	22
Caelo	Hydrocortisone	18091525	44
Caelo	Hydrocortisone	180915252	1
Caelo	Hydrocortisone	18091526	6
Caelo	Hydrocortisone	18091528	22
Caelo	Hydrocortisone	18091530	1
Caelo	Hydrocortisone	18091531	18
Caelo	Hydrocortisone	18091531x2	1
Caelo	Hydrocortisone	180915321	1
Caelo	Hydrocortisone	180921531	1
Caelo	Hydrocortisone	18121713	1
Caelo	Hydrocortisone	1824311	1
Caelo	Hydrocortisone	1832243006	1
Caelo	Hydrocortisone	18323006	1
Caelo	Hydrocortisone	18324207	1
Caelo	Hydrocortisone	183243002	58
Caelo	Hydrocortisone	183243003	7
Caelo	Hydrocortisone	183243004	19
Caelo	Hydrocortisone	183243006	54
Caelo	Hydrocortisone	18324301	32
Caelo	Hydrocortisone	18324302	28
Caelo	Hydrocortisone	18324303	6
Caelo	Hydrocortisone	18324306	34
Caelo	Hydrocortisone	18324307	31
Caelo	Hydrocortisone	18324308	24
Caelo	Hydrocortisone	18324310	9
Caelo	Hydrocortisone	18324311	27
Caelo	Hydrocortisone	186324307	1
Caelo	Hydrocortisone	1891528	1
Caelo	Hydrocortisone	1907151621	1
Caelo	Hydrocortisone	19224002	1
Caelo	Hydrocortisone	19224100	1
Caelo	Hydrocortisone	192241002	5
Caelo	Hydrocortisone	192241004	15
Caelo	Hydrocortisone	192241005	30
Caelo	Hydrocortisone	192241007	24
Caelo	Hydrocortisone	192241008	70
Caelo	Hydrocortisone	200004116007	2
Caelo	Hydrocortisone	20004106005	1
Caelo	Hydrocortisone	200041116003	1
Caelo	Hydrocortisone	20004116001	35
Caelo	Hydrocortisone	20004116002	11
Caelo	Hydrocortisone	20004116003	29
Caelo	Hydrocortisone	20004116004	32
Caelo	Hydrocortisone	20004116005	22
Caelo	Hydrocortisone	20004116006	24
Caelo	Hydrocortisone	20004116007	16
Caelo	Hydrocortisone	20004278004	1
Caelo	Hydrocortisone	2004116006	1
Caelo	Hydrocortisone	200411606	1
Caelo	Hydrocortisone	2013U-01719	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hydrocortisone	2100115007	1
Caelo	Hydrocortisone	21001215003	3
Caelo	Hydrocortisone	21001215004	15
Caelo	Hydrocortisone	21001215005	37
Caelo	Hydrocortisone	21001215006	23
Caelo	Hydrocortisone	21001215007	24
Caelo	Hydrocortisone	21001215009	1
Caelo	Hydrocortisone	21001215010	28
Caelo	Hydrocortisone	21001215011	12
Caelo	Hydrocortisone	21001215013	29
Caelo	Hydrocortisone	21001215014	20
Caelo	Hydrocortisone	21001215015	7
Caelo	Hydrocortisone	21001215017	10
Caelo	Hydrocortisone	21001215018	13
Caelo	Hydrocortisone	21001215019	13
Caelo	Hydrocortisone	21001215020	12
Caelo	Hydrocortisone	21001215021	23
Caelo	Hydrocortisone	21001215023	3
Caelo	Hydrocortisone	21001215026	2
Caelo	Hydrocortisone	21001215027	2
Caelo	Hydrocortisone	21001215029	1
Caelo	Hydrocortisone	2100125014	1
Caelo	Hydrocortisone	210012515010	1
Caelo	Hydrocortisone	2100215013	1
Caelo	Hydrocortisone	210922(20004116002)	1
Caelo	Hydrocortisone	21101303	1
Caelo	Hydrocortisone	211029(21001215003)	1
Caelo	Hydrocortisone	211115(21001215003)	1
Caelo	Hydrocortisone	211123(21001215003)	2
Caelo	Hydrocortisone	211130(21001215003)	1
Caelo	Hydrocortisone	211227(21001215003)	1
Caelo	Hydrocortisone	2180917/16255608	1
Caelo	Hydrocortisone	220037789006	1
Caelo	Hydrocortisone	22003779005	2
Caelo	Hydrocortisone	22003779008	1
Caelo	Hydrocortisone	220118(21001215003)	1
Caelo	Hydrocortisone	220120	1
Caelo	Hydrocortisone	220127	1
Caelo	Hydrocortisone	220210(21001215003)	1
Caelo	Hydrocortisone	220413(21001215003)	1
Caelo	Hydrocortisone	2205003-01	4
Caelo	Hydrocortisone	220510(21001215009)	1
Caelo	Hydrocortisone	220519(21001215003)	1
Caelo	Hydrocortisone	220905(21001215015)	1
Caelo	Hydrocortisone	260416v4	1
Caelo	Hydrocortisone	27101801	1
Caelo	Hydrocortisone	2760	1
Caelo	Hydrocortisone	3081604	1
Caelo	Hydrocortisone	31032014D	1
Caelo	Hydrocortisone	3110396	1
Caelo	Hydrocortisone	3110456	1
Caelo	Hydrocortisone	39/AKD17	1
Caelo	Hydrocortisone	3912Q-01719	1
Caelo	Hydrocortisone	4817Q-01719	1
Caelo	Hydrocortisone	7082004	1
Caelo	Hydrocortisone	7101301	1
Caelo	Hydrocortisone	8041701	1
Caelo	Hydrocortisone	810911	1
Caelo	Hydrocortisone	8717	1
Caelo	Hydrocortisone	9271205	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hydrocortisone	B02-2005104	1
Caelo	Hydrocortisone	caelo	1
Caelo	Hydrocortisone	Caelo21001215003	2
Caelo	Hydrocortisone	K05B20160909	1
Caeol/Noweda	Hydrocortisone	16095212	1
Caeolo/Krieger	Hydrocortisone	17119406	1
Caesar & Lorenz GmbH	Hydrocortisone	15181004	1
Caesar & Lorenz	Hydrocortisone	21001215026	1
Caesar & Loretz /Phönix	Hydrocortisone	21001215003	1
Caesar & Loretz /Sanacorp	Hydrocortisone	21001215011	2
Caesar & Loretz GmbH...	Hydrocortisone	21001215006	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215014	1
Caesar & Loretz GmbH...	Hydrocortisone	183243006	1
Caesar & Loretz GmbH...	Hydrocortisone	20004116001	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215021	1
Caesar & Loretz GmbH...	Hydrocortisone	18324306	1
Caesar & Loretz GmbH...	Hydrocortisone	20004116001	1
Caesar & Loretz GmbH...	Hydrocortisone	20004116004	1
Caesar & Loretz GmbH...	Hydrocortisone	192241008	1
Caesar & Loretz GmbH...	Hydrocortisone	183243006	1
Caesar & Loretz GmbH...	Hydrocortisone	18324307	1
Caesar & Loretz GmbH...	Hydrocortisone	18324308	1
Caesar & Loretz GmbH...	Hydrocortisone	192241008	1
Caesar & Loretz GmbH...	Hydrocortisone	20004116003	1
Caesar & Loretz GmbH...	Hydrocortisone	192241008	1
Caesar & Loretz GmbH...	Hydrocortisone	18324211	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215005	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215023	1
Caesar & Loretz GmbH...	Hydrocortisone	20004116002	1
Caesar & Loretz GmbH...	Hydrocortisone	183243002	1
Caesar & Loretz GmbH...	Hydrocortisone	18324311	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215009	1
Caesar & Loretz GmbH/AEP	Hydrocortisone	18091525	1
Caesar & Loretz GmbH/AEP	Hydrocortisone	21001215011	1
Caesar & Loretz GmbH/AHD	Hydrocortisone	20004116004	1
Caesar & Loretz GmbH/AHD	Hydrocortisone	21001215011	1
Caesar & Loretz GmbH...	Hydrocortisone	20004116001	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215007	1
Caesar & Loretz GmbH...	Hydrocortisone	183243006	1
Caesar & Loretz GmbH...	Hydrocortisone	18091508	1
Caesar & Loretz GmbH...	Hydrocortisone	183243003	1
Caesar & Loretz GmbH...	Hydrocortisone	192241008	1
Caesar & Loretz GmbH/G	Hydrocortisone	192241007	1
Caesar & Loretz GmbH/G	Hydrocortisone	21001215004	1
Caesar & Loretz GmbH/G	Hydrocortisone	21001215011	1
Caesar & Loretz GmbH/GEHE	Hydrocortisone	192241008	1
Caesar & Loretz GmbH/Gehe	Hydrocortisone	20004116005	1
Caesar & Loretz GmbH/Gehe	Hydrocortisone	21001215004	2
Caesar & Loretz GmbH/Gehe	Hydrocortisone	21001215023	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215005	2
Caesar & Loretz GmbH...	Hydrocortisone	18324302	1
Caesar & Loretz GmbH...	Hydrocortisone	20004116006	2
Caesar & Loretz GmbH...	Hydrocortisone	21001215006	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215020	2
Caesar & Loretz GmbH...	Hydrocortisone	18091524	1
Caesar & Loretz GmbH...	Hydrocortisone	183243004	1
Caesar & Loretz GmbH...	Hydrocortisone	18324306	1
Caesar & Loretz GmbH...	Hydrocortisone	192241008	1
Caesar & Loretz GmbH...	Hydrocortisone	20004116005	1
Caesar & Loretz GmbH...	Hydrocortisone	20004116006	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Hydrocortisone	21001215004	2
Caesar & Loretz GmbH...	Hydrocortisone	21001215007	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215010	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215013	1
Caesar & Loretz GmbH/Kehr	Hydrocortisone	183243006	1
Caesar & Loretz GmbH/Kehr	Hydrocortisone	18324301	1
Caesar & Loretz GmbH/Kehr	Hydrocortisone	18324306	1
Caesar & Loretz GmbH/Kehr	Hydrocortisone	18324308	1
Caesar & Loretz GmbH/Kehr	Hydrocortisone	20004116007	1
Caesar & Loretz GmbH...	Hydrocortisone	183243002	2
Caesar & Loretz GmbH...	Hydrocortisone	20004116001	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215005	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215006	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215010	1
Caesar & Loretz GmbH...	Hydrocortisone	183243003	2
Caesar & Loretz GmbH...	Hydrocortisone	18324302	1
Caesar & Loretz GmbH...	Hydrocortisone	192241005	2
Caesar & Loretz GmbH...	Hydrocortisone	20004116006	1
Caesar & Loretz GmbH...	Hydrocortisone	20004116007	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215020	1
Caesar & Loretz GmbH/Otto	Hydrocortisone	18324307	1
Caesar & Loretz GmbH...	Hydrocortisone	20004116002	2
Caesar & Loretz GmbH/Phoe	Hydrocortisone	20004116004	1
Caesar & Loretz GmbH...	Hydrocortisone	18324302	1
Caesar & Loretz GmbH...	Hydrocortisone	20004116003	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215010	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215021	1
Caesar & Loretz GmbH...	Hydrocortisone	18091520	1
Caesar & Loretz GmbH...	Hydrocortisone	183243003	2
Caesar & Loretz GmbH...	Hydrocortisone	183243006	1
Caesar & Loretz GmbH...	Hydrocortisone	18324301	1
Caesar & Loretz GmbH...	Hydrocortisone	192241005	1
Caesar & Loretz GmbH...	Hydrocortisone	192241008	1
Caesar & Loretz GmbH...	Hydrocortisone	20004116002	1
Caesar & Loretz GmbH...	Hydrocortisone	20004116003	1
Caesar & Loretz GmbH...	Hydrocortisone	20004116005	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215003	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215006	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215007	2
Caesar & Loretz GmbH...	Hydrocortisone	21001215013	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215014	1
Caesar & Loretz GmbH/Sa	Hydrocortisone	18324302	1
Caesar & Loretz GmbH/Sana	Hydrocortisone	20004116004	1
Caesar & Loretz GmbH/Sana	Hydrocortisone	21001215006	1
Caesar & Loretz GmbH...	Hydrocortisone	183243002	1
Caesar & Loretz GmbH...	Hydrocortisone	192241004	1
Caesar & Loretz GmbH...	Hydrocortisone	192241008	1
Caesar & Loretz GmbH...	Hydrocortisone	20004116003	3
Caesar & Loretz GmbH...	Hydrocortisone	21001215007	2
Caesar & Loretz GmbH...	Hydrocortisone	21001215013	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215014	1
Caesar & Loretz GmbH...	Hydrocortisone	21001215017	1
Caesar & Loretz GmbH	Hydrocortisone	12167010	1
Caesar & Loretz GmbH	Hydrocortisone	13069506	1
Caesar & Loretz GmbH	Hydrocortisone	13069507	1
Caesar & Loretz GmbH	Hydrocortisone	15021107	1
Caesar & Loretz GmbH	Hydrocortisone	15181012	1
Caesar & Loretz GmbH	Hydrocortisone	16004612	1
Caesar & Loretz GmbH	Hydrocortisone	17256605	1
Caesar & Loretz GmbH	Hydrocortisone	17351205	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Hydrocortisone	17351210	3
Caesar & Loretz GmbH	Hydrocortisone	18091505	1
Caesar & Loretz GmbH	Hydrocortisone	18091506	4
Caesar & Loretz GmbH	Hydrocortisone	18091507	1
Caesar & Loretz GmbH	Hydrocortisone	18091519	6
Caesar & Loretz GmbH	Hydrocortisone	18091520	10
Caesar & Loretz GmbH	Hydrocortisone	18091524	3
Caesar & Loretz GmbH	Hydrocortisone	18091525	6
Caesar & Loretz GmbH	Hydrocortisone	18091526	3
Caesar & Loretz GmbH	Hydrocortisone	18091528	6
Caesar & Loretz GmbH	Hydrocortisone	18091531	4
Caesar & Loretz GmbH	Hydrocortisone	183243002	11
Caesar & Loretz GmbH	Hydrocortisone	183243004	13
Caesar & Loretz GmbH	Hydrocortisone	183243006	12
Caesar & Loretz GmbH	Hydrocortisone	18324301	6
Caesar & Loretz GmbH	Hydrocortisone	18324302	12
Caesar & Loretz GmbH	Hydrocortisone	18324303	1
Caesar & Loretz GmbH	Hydrocortisone	18324306	13
Caesar & Loretz GmbH	Hydrocortisone	18324307	13
Caesar & Loretz GmbH	Hydrocortisone	18324308	8
Caesar & Loretz GmbH	Hydrocortisone	18324310	4
Caesar & Loretz GmbH	Hydrocortisone	18324311	9
Caesar & Loretz GmbH	Hydrocortisone	192241002	8
Caesar & Loretz GmbH	Hydrocortisone	192241003	1
Caesar & Loretz GmbH	Hydrocortisone	192241004	1
Caesar & Loretz GmbH	Hydrocortisone	192241005	3
Caesar & Loretz GmbH	Hydrocortisone	192241007	11
Caesar & Loretz GmbH	Hydrocortisone	192241008	20
Caesar & Loretz GmbH	Hydrocortisone	19K05-B02-195614	1
Caesar & Loretz GmbH	Hydrocortisone	20000978010	1
Caesar & Loretz GmbH	Hydrocortisone	20004116001	16
Caesar & Loretz GmbH	Hydrocortisone	20004116002	5
Caesar & Loretz GmbH	Hydrocortisone	20004116003	15
Caesar & Loretz GmbH	Hydrocortisone	20004116004	12
Caesar & Loretz GmbH	Hydrocortisone	20004116005	2
Caesar & Loretz GmbH	Hydrocortisone	20004116006	15
Caesar & Loretz GmbH	Hydrocortisone	20004116007	7
Caesar & Loretz GmbH	Hydrocortisone	20B17-B02-200514	1
Caesar & Loretz GmbH	Hydrocortisone	21001215003	2
Caesar & Loretz GmbH	Hydrocortisone	21001215004	10
Caesar & Loretz GmbH	Hydrocortisone	21001215005	10
Caesar & Loretz GmbH	Hydrocortisone	21001215006	6
Caesar & Loretz GmbH	Hydrocortisone	21001215007	7
Caesar & Loretz GmbH	Hydrocortisone	21001215009	2
Caesar & Loretz GmbH	Hydrocortisone	21001215010	10
Caesar & Loretz GmbH	Hydrocortisone	21001215011	9
Caesar & Loretz GmbH	Hydrocortisone	21001215013	7
Caesar & Loretz GmbH	Hydrocortisone	21001215014	9
Caesar & Loretz GmbH	Hydrocortisone	21001215015	2
Caesar & Loretz GmbH	Hydrocortisone	21001215016	1
Caesar & Loretz GmbH	Hydrocortisone	21001215017	1
Caesar & Loretz GmbH	Hydrocortisone	21001215018	2
Caesar & Loretz GmbH	Hydrocortisone	21001215019	9
Caesar & Loretz GmbH	Hydrocortisone	21001215020	5
Caesar & Loretz GmbH	Hydrocortisone	21001215021	5
Caesar & Loretz GmbH	Hydrocortisone	21001215023	5
Caesar & Loretz GmbH	Hydrocortisone	21001215028	1
Caesar & Loretz GmbH	Hydrocortisone	21001215029	1
Caesar & Loretz GmbH	Hydrocortisone	21001215030	2
Caesar & Loretz GmbH	Hydrocortisone	21001215035	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Hydrocortisone	22003779004	1
Caesar & Loretz GmbH	Hydrocortisone	22003779006	1
Caesar & Loretz GmbH	Hydrocortisone	B02-1956104	1
Caesar & Loretz GmbH...	Hydrocortisone	192241007	1
Caesar & Loretz Hild...	Hydrocortisone	192241004	1
Caesar & Loretz Hilden	Hydrocortisone	18091520	1
Caesar & Loretz Hilden	Hydrocortisone	183243002	1
Caesar & Loretz Hilden	Hydrocortisone	183243006	1
Caesar & Loretz Hilden	Hydrocortisone	18324306	1
Caesar & Loretz/ Gei...	Hydrocortisone	18091520	1
Caesar & Loretz/Geil...	Hydrocortisone	18091528	1
Caesar & Loretz/Noweda	Hydrocortisone	192241005	1
Caesar & Loretz/Phoenix	Hydrocortisone	21001215006	1
Caesar & Loretz	Hydrocortisone	16095201	1
Caesar & Loretz	Hydrocortisone	16255603	1
Caesar & Loretz	Hydrocortisone	17256603	2
Caesar & Loretz	Hydrocortisone	192241008	1
Caesar / Phönix 22.0...	Hydrocortisone	20004116007	1
Caesar&Lorenz	Hydrocortisone	20004116003	1
Caesar&Loretz GmbH,A...	Hydrocortisone	16272305	1
Caesar&Loretz GmbH	Hydrocortisone	12104308	1
Caesar&Loretz GmbH	Hydrocortisone	21001215020	1
Caesar&loretz,Phoenix	Hydrocortisone	15021105	1
Caesar&loretz,Phoenix	Hydrocortisone	15181004	1
Caesar/Alliance Heal...	Hydrocortisone	20004116004	1
Caleo/ Noweda	Hydrocortisone	17351203	2
Cealo / Anzag	Hydrocortisone	220322(21001215003)	1
Cealo / Anzag	Hydrocortisone	220419(21001215003)	1
Cealo / Anzag	Hydrocortisone	220531(21001215003)	1
Cealo / Anzag	Hydrocortisone	220712(21001215003)	1
Cealo, Anzag 26.08.19	Hydrocortisone	18091528	1
Cealo/ Anzag	Hydrocortisone	16095210	1
Cealo/ Noweda	Hydrocortisone	17351209	1
Cealo/Jenne	Hydrocortisone	211019(21001215003)	2
Cealo/Jenne	Hydrocortisone	211104(20004116005)	2
Cealo/Sanacorp	Hydrocortisone	20004116004	1
Cealo	Hydrocortisone	16004612	1
Cealo	Hydrocortisone	17119405	1
Cealo	Hydrocortisone	18091503	1
Cealo	Hydrocortisone	18091505	1
Cealo	Hydrocortisone	192241004	1
Celo/AHD	Hydrocortisone	18091506	1
Delta	Hydrocortisone	16H01-B01-326071	1
Ebert & Jacobi	Hydrocortisone	1509029-01	1
Eu Rho/gehe	Hydrocortisone	1611016-01	1
EuRho / Noweda	Hydrocortisone	1906033-01	1
EuRho 12.03.2013 Anzag	Hydrocortisone	1112030-01	1
EuRho/ Anzag	Hydrocortisone	113(1906033-01)	1
Eurho/ Phönix	Hydrocortisone	180200901	1
EuRho/AHD	Hydrocortisone	1802009-01	1
EuRho/GEHE	Hydrocortisone	1611016-01	1
EuRho/Jenne	Hydrocortisone	1906033-01	1
EuRho/Noweda	Hydrocortisone	1611016-01	1
Eurho/Phönix	Hydrocortisone	210100302	1
EuRho	Hydrocortisone	1107005-02	1
EuRho	Hydrocortisone	1202032-01	1
EuRho	Hydrocortisone	1204037-01	1
EuRho	Hydrocortisone	1405001-01	3
EuRho	Hydrocortisone	1509029-01	1
EuRho	Hydrocortisone	1611016-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho	Hydrocortisone	180200-01	1
EuRho	Hydrocortisone	2101003-01	11
Euro / AHD	Hydrocortisone	1906033-01	1
EURO / Gehe	Hydrocortisone	1405001-01	1
Euro Gehe	Hydrocortisone	1611016-01	1
Euro Gehe	Hydrocortisone	1802009-01	1
Euro OT/Anzag	Hydrocortisone	1611016-01	3
Euro OTC	Hydrocortisone	100(1906033-01)	1
Euro OTC	Hydrocortisone	101(1906033-01)	1
Euro OTC	Hydrocortisone	102(1906033-01)	1
Euro OTC	Hydrocortisone	103(1906033-01)	1
Euro OTC	Hydrocortisone	104(1906033)	1
Euro OTC	Hydrocortisone	105(1906033-01)	1
Euro OTC	Hydrocortisone	106(1906033-01)	1
Euro OTC	Hydrocortisone	107(1906033-01)	1
Euro OTC	Hydrocortisone	108(1906033-01)	1
Euro OTC	Hydrocortisone	1082009-01	1
Euro OTC	Hydrocortisone	109(1906033-01)	1
Euro OTC	Hydrocortisone	1096033-01	1
Euro OTC	Hydrocortisone	110(1906033-01)	1
Euro OTC	Hydrocortisone	1107005-01	1
Euro OTC	Hydrocortisone	1107005-02	3
Euro OTC	Hydrocortisone	1107005-03	8
Euro OTC	Hydrocortisone	111(1906033-01)	1
Euro OTC	Hydrocortisone	1112030-01	9
Euro OTC	Hydrocortisone	112(1906033-01)	1
Euro OTC	Hydrocortisone	11611016-01	1
Euro OTC	Hydrocortisone	119(2101003-01)	1
Euro OTC	Hydrocortisone	1202032-01	3
Euro OTC	Hydrocortisone	120403701	3
Euro OTC	Hydrocortisone	1204037-01	26
Euro OTC	Hydrocortisone	1204307-01	1
Euro OTC	Hydrocortisone	12060018-01	1
Euro OTC	Hydrocortisone	1206018-01	23
Euro OTC	Hydrocortisone	120618-01	1
Euro OTC	Hydrocortisone	1405001	1
Euro OTC	Hydrocortisone	1405001-01	2
Euro OTC	Hydrocortisone	1408023-01	4
Euro OTC	Hydrocortisone	1501034	1
Euro OTC	Hydrocortisone	1501034-01	10
Euro OTC	Hydrocortisone	1505010601	1
Euro OTC	Hydrocortisone	150501601	1
Euro OTC	Hydrocortisone	1505016-01	30
Euro OTC	Hydrocortisone	15050-16-01	1
Euro OTC	Hydrocortisone	150516-01	1
Euro OTC	Hydrocortisone	150902	1
Euro OTC	Hydrocortisone	1509029	1
Euro OTC	Hydrocortisone	150902901	2
Euro OTC	Hydrocortisone	1509029-01	42
Euro OTC	Hydrocortisone	150929-01	1
Euro OTC	Hydrocortisone	15278703	1
Euro OTC	Hydrocortisone	157015	2
Euro OTC	Hydrocortisone	16004612	1
Euro OTC	Hydrocortisone	161016-01	1
Euro OTC	Hydrocortisone	16110016-01	1
Euro OTC	Hydrocortisone	1611016	1
Euro OTC	Hydrocortisone	161101601	3
Euro OTC	Hydrocortisone	1611016-01	75
Euro OTC	Hydrocortisone	161116-01	1
Euro OTC	Hydrocortisone	16272305	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Hydrocortisone	16272311	1
Euro OTC	Hydrocortisone	1708006-01	1
Euro OTC	Hydrocortisone	17119402	1
Euro OTC	Hydrocortisone	17119403	2
Euro OTC	Hydrocortisone	17256603	1
Euro OTC	Hydrocortisone	17351202	1
Euro OTC	Hydrocortisone	1801009-01	1
Euro OTC	Hydrocortisone	1802008-01	1
Euro OTC	Hydrocortisone	1802009	1
Euro OTC	Hydrocortisone	180200901	4
Euro OTC	Hydrocortisone	1802009-01	84
Euro OTC	Hydrocortisone	18091501	1
Euro OTC	Hydrocortisone	18091506	1
Euro OTC	Hydrocortisone	181102182	1
Euro OTC	Hydrocortisone	1906033	2
Euro OTC	Hydrocortisone	190603301	1
Euro OTC	Hydrocortisone	1906033-01	91
Euro OTC	Hydrocortisone	190633-01	3
Euro OTC	Hydrocortisone	19069033-01	1
Euro OTC	Hydrocortisone	2019Q-01719	1
Euro OTC	Hydrocortisone	2101003-001	1
Euro OTC	Hydrocortisone	210100301	1
Euro OTC	Hydrocortisone	2101003-01	39
Euro OTC	Hydrocortisone	2101003-02	8
Euro OTC	Hydrocortisone	210818A	1
Euro OTC	Hydrocortisone	210826	1
Euro OTC	Hydrocortisone	210906(2101003-01)	1
Euro OTC	Hydrocortisone	211118(2101003-01)	1
Euro OTC	Hydrocortisone	2205003-01	5
Euro OTC	Hydrocortisone	29011504	1
Euro OTC	Hydrocortisone	3817A-01719	1
Euro OTC	Hydrocortisone	4091510	1
Euro OTC	Hydrocortisone	4112A-01719	1
Euro OTC	Hydrocortisone	4616U-01719	1
Euro OTC	Hydrocortisone	6051502	1
Euro OTC	Hydrocortisone	715Q-01719	1
Euro OTC	Hydrocortisone	79(1802009-01)	1
Euro OTC	Hydrocortisone	80(1802009-01)	1
Euro OTC	Hydrocortisone	81(1802009-01)	1
Euro OTC	Hydrocortisone	82(1802009-01)	1
Euro OTC	Hydrocortisone	8639285	1
Euro OTC	Hydrocortisone	906033-01	1
Euro OTC	Hydrocortisone	K05B20160909	1
Euro OTC	Hydrocortisone	K05B20180323	1
Euro OTC	Hydrocortisone	K05M20170313	1
Euro OTC	Hydrocortisone	k05m20201110	1
Euro OTC	Hydrocortisone	L39844	1
Euro/ Phönix	Hydrocortisone	1509029-01	1
Euro/Phönix	Hydrocortisone	210100301	1
Euro/Sanacorp	Hydrocortisone	1906033-01	2
Fagro/Otto Geilenkirchen	Hydrocortisone	19k05-b02-195614	1
Fagron	Hydrocortisone		2
Fagron	Hydrocortisone	11021403	1
Fagron	Hydrocortisone	114(19K05-B02-195615)	1
Fagron	Hydrocortisone	115(19K015-0004)	1
Fagron	Hydrocortisone	116(19K05-B02-195615)	1
Fagron	Hydrocortisone	117(19K05-B02-195615)	1
Fagron	Hydrocortisone	11K18-N01	2
Fagron	Hydrocortisone	12/25-N01	1
Fagron	Hydrocortisone	1204037-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Hydrocortisone	120601801	1
Fagron	Hydrocortisone	12091401	1
Fagron	Hydrocortisone	12104304	1
Fagron	Hydrocortisone	12119303	1
Fagron	Hydrocortisone	12G19-N01	2
Fagron	Hydrocortisone	12I25-N01	2
Fagron	Hydrocortisone	13341510	1
Fagron	Hydrocortisone	13H08-B01-285469	1
Fagron	Hydrocortisone	13H08-B01-285472	1
Fagron	Hydrocortisone	13H08B01285473	1
Fagron	Hydrocortisone	13H08-B01-285473	1
Fagron	Hydrocortisone	13H08-B01-28571	1
Fagron	Hydrocortisone	13K22-B01-288282	1
Fagron	Hydrocortisone	13K22-B01-288283	1
Fagron	Hydrocortisone	13K22-B01-288284	3
Fagron	Hydrocortisone	14/05-B02-300227	2
Fagron	Hydrocortisone	14/05-BO2-300227	1
Fagron	Hydrocortisone	14B04-B02	2
Fagron	Hydrocortisone	14B04-B02-293422	3
Fagron	Hydrocortisone	14B04-B02-293423	4
Fagron	Hydrocortisone	14B04-B02-293424	6
Fagron	Hydrocortisone	14I05-B02	2
Fagron	Hydrocortisone	14I05-B02-300227	1
Fagron	Hydrocortisone	14I05-B02-300228	1
Fagron	Hydrocortisone	14I05-B02-300229	1
Fagron	Hydrocortisone	14l05-B02-300227	1
Fagron	Hydrocortisone	14l05-B02-300228	1
Fagron	Hydrocortisone	15/25-B01-313084	1
Fagron	Hydrocortisone	15/25-B01-318727	1
Fagron	Hydrocortisone	15015	1
Fagron	Hydrocortisone	1509029-01	1
Fagron	Hydrocortisone	15D14-B02	1
Fagron	Hydrocortisone	15D14-B02-311696	5
Fagron	Hydrocortisone	15I04-B03-315021	1
Fagron	Hydrocortisone	15I25-B01-318727	1
Fagron	Hydrocortisone	15l25-B01-318486	1
Fagron	Hydrocortisone	16272311	1
Fagron	Hydrocortisone	16A19-B06	1
Fagron	Hydrocortisone	16A19-B06-320970	20
Fagron	Hydrocortisone	16A19-B06-321981	2
Fagron	Hydrocortisone	16A19-B06-321982	1
Fagron	Hydrocortisone	16H01-B01	1
Fagron	Hydrocortisone	16H01-B01-324891	1
Fagron	Hydrocortisone	16H01-B01-324944	5
Fagron	Hydrocortisone	16H01-B01-326071	3
Fagron	Hydrocortisone	16J26-B04	1
Fagron	Hydrocortisone	16J26-B04-328188	1
Fagron	Hydrocortisone	16J26-B04-329419	1
Fagron	Hydrocortisone	16j26-b04-330339	1
Fagron	Hydrocortisone	16J26-B04-330340	2
Fagron	Hydrocortisone	17/12-b05-344220	1
Fagron	Hydrocortisone	17/12-B05-344220	2
Fagron	Hydrocortisone	17/12-B05-345540	1
Fagron	Hydrocortisone	17/12-Bos-344220	1
Fagron	Hydrocortisone	17119405	1
Fagron	Hydrocortisone	17-12B05-342611	1
Fagron	Hydrocortisone	1712-B05-345540	2
Fagron	Hydrocortisone	17256604	1
Fagron	Hydrocortisone	17351205	1
Fagron	Hydrocortisone	17c13-B06	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Hydrocortisone	17C13-B06	1
Fagron	Hydrocortisone	17C13-B06-333045	4
Fagron	Hydrocortisone	17E10-B04	2
Fagron	Hydrocortisone	17E10-B04-334857	5
Fagron	Hydrocortisone	17E-10-B04-334857	1
Fagron	Hydrocortisone	17E10-B04-334858	4
Fagron	Hydrocortisone	17e10-b04-335056	1
Fagron	Hydrocortisone	17E10-B04-335056	3
Fagron	Hydrocortisone	17E10B04335656	1
Fagron	Hydrocortisone	17E10-B04-335656	2
Fagron	Hydrocortisone	17E10-B04-336435	7
Fagron	Hydrocortisone	17E10-B04-336436	2
Fagron	Hydrocortisone	17g25-b02-340864	1
Fagron	Hydrocortisone	17G25-B02-340864	2
Fagron	Hydrocortisone	17G25-B02-340865	1
Fagron	Hydrocortisone	17I12-B05	1
Fagron	Hydrocortisone	17I12-B05-344220	2
Fagron	Hydrocortisone	17I12-B05-34554	1
Fagron	Hydrocortisone	18091501	1
Fagron	Hydrocortisone	18B21-B07	2
Fagron	Hydrocortisone	18B21-B07-348430	3
Fagron	Hydrocortisone	18B21-B07-348431	4
Fagron	Hydrocortisone	18B21-B07-348432	3
Fagron	Hydrocortisone	18B21-B07-360920	1
Fagron	Hydrocortisone	19051403	1
Fagron	Hydrocortisone	19K05-802-195615	1
Fagron	Hydrocortisone	19K05-B02-195613	3
Fagron	Hydrocortisone	19K05-B02-195614	3
Fagron	Hydrocortisone	19k05-b02-195615	1
Fagron	Hydrocortisone	19K05-B02-195615	6
Fagron	Hydrocortisone	20B17-802-2000542	1
Fagron	Hydrocortisone	20B17-B02-200514	4
Fagron	Hydrocortisone	20B17-B02-200543	4
Fagron	Hydrocortisone	20B17-B02-200544	8
Fagron	Hydrocortisone	20B17-B02-200571	2
Fagron	Hydrocortisone	21011003-02	1
Fagron	Hydrocortisone	-21965000	1
Fagron	Hydrocortisone	22E09-B02-219650	1
Fagron	Hydrocortisone	23D06-B02-234497	1
Fagron	Hydrocortisone	2OB17-BO2-200543	1
Fagron	Hydrocortisone	5061304	1
Fagron	Hydrocortisone	BO-20051004	1
Fagron	Hydrocortisone	BO2-2005104	1
Fagron	Hydrocortisone	BO2-2005403	3
Fagron	Hydrocortisone	BO2-1956104	1
Fagron	Hydrocortisone	K05B20130407M	1
Fagron	Hydrocortisone	K05B20131101	1
Fagron	Hydrocortisone	K05M20170702	1
Fagron	Hydrocortisone	PH132	1
Fagron	Hydrocortisone	T3319	1
Fargo/Anzag	Hydrocortisone	17E10-B04-335056	1
Fargon	Hydrocortisone	17E10-B04-334858	1
fargon	Hydrocortisone	T3325	1
fargron	Hydrocortisone	13K22-B01-288284	1
Fiebig	Hydrocortisone	1509029-01	2
Fiebig	Hydrocortisone	16095207	1
Fiebig	Hydrocortisone	16095210	1
Fiebig	Hydrocortisone	17119402	2
Fiebig	Hydrocortisone	17256602	1
Fiebig	Hydrocortisone	18091520	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fiebig	Hydrocortisone	18091525	1
Fiebig	Hydrocortisone	18091528	1
Finteler Apotheke	Hydrocortisone	1611016-01	3
Fischar/ Anzag	Hydrocortisone	118(20B17-B02-200544)	1
Fragon/Anzag	Hydrocortisone	19K05-b02-195615	1
Fragon/Sanacorp	Hydrocortisone	17E10-B04-335056	1
Gatt-Koller	Hydrocortisone	1804169	1
Gatt-Koller	Hydrocortisone	20172187	1
Gatt-Koller	Hydrocortisone	22J00274	1
GEHE 03.05.2014	Hydrocortisone	13155605	1
GEHE 14.04.2014	Hydrocortisone	13069509	1
Gehe,27.0415	Hydrocortisone	14301310	1
Gehe/EuRho	Hydrocortisone	19060033-01	1
Gehe/Europharm	Hydrocortisone	1802009-01	1
Gehe/Jenne	Hydrocortisone	20004116001	1
Gehe	Hydrocortisone	1206018-01	2
Gehe	Hydrocortisone	12104304	3
Gehe	Hydrocortisone	13069510	1
Gehe	Hydrocortisone	13341510	1
Gehe	Hydrocortisone	13H08-B01-285469	1
Gehe	Hydrocortisone	13H08-B01-285471	1
Gehe	Hydrocortisone	1405001-01	1
Gehe	Hydrocortisone	1501034-01	1
Gehe	Hydrocortisone	1509029-01	1
Gehe	Hydrocortisone	1611016-01	1
gehe	Hydrocortisone	16255607	1
Gehe	Hydrocortisone	16255607	1
Gehe	Hydrocortisone	16255608	1
Gehe	Hydrocortisone	16272306	1
GEHE	Hydrocortisone	16272311	1
Gehe	Hydrocortisone	17256604	1
Gehe	Hydrocortisone	17351203	1
Gehe	Hydrocortisone	17351206	1
Gehe	Hydrocortisone	17E10-B04-335656	1
Gehe	Hydrocortisone	1802009-01	1
Gehe	Hydrocortisone	18091502	2
Gehe	Hydrocortisone	18091521	1
Gehe	Hydrocortisone	183243004	1
Gehe	Hydrocortisone	18324301	2
GEHE	Hydrocortisone	18324301	1
Gehe	Hydrocortisone	18324303	1
Gehe	Hydrocortisone	18324310	1
Gehe	Hydrocortisone	1906033-01	1
Gehe	Hydrocortisone	192241002	1
Gehe	Hydrocortisone	2004116006	1
Gehe	Hydrocortisone	21001215003	1
Gehe	Hydrocortisone	21001215013	1
Gehe	Hydrocortisone	21001215019	1
Gehe	Hydrocortisone	21001215021	1
Gehe	Hydrocortisone	21001215027	2
Gehe	Hydrocortisone	21001215035	3
Gehe	Hydrocortisone	2101003-01	1
Gehe	Hydrocortisone	22003779004	1
GEHE	Hydrocortisone	2205003-01	1
Ge-Hh	Hydrocortisone	192241002	1
Geilenkirchen	Hydrocortisone	1611016-01	1
Geilenkirchen	Hydrocortisone	20004116007	1
Henan Lihua Pharm/AHD	Hydrocortisone	18B21-B07-348430	1
Henan Lihua Pharmace...	Hydrocortisone	1906033-01	1
Henan/Noweda	Hydrocortisone	K05M20170408	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Henan/Noweda	Hydrocortisone	K05M20170701	1
Jenne	Hydrocortisone	18324307	2
Jenne	Hydrocortisone	22003779004	1
Jenne	Hydrocortisone	22003779005	1
Kehr	Hydrocortisone	16095213	1
Kehr	Hydrocortisone	17119407	1
Kehr	Hydrocortisone	17256602	1
Kehr	Hydrocortisone	20004116003	2
Kehr	Hydrocortisone	21001215026	2
Kehr	Hydrocortisone	21001215027	2
Kehr	Hydrocortisone	21001215029	1
Kehr	Hydrocortisone	22003779004	2
Kehr	Hydrocortisone	2205003-01	2
Klenk	Hydrocortisone	12167007	1
L12	Hydrocortisone	16H01-B01-326071	2
L12	Hydrocortisone	1802009-01	1
Laborchemie Apolda/Phönix	Hydrocortisone	15181004	1
Midas	Hydrocortisone	17256602	1
Midas	Hydrocortisone	18091519	1
Nachprüfung 2312	Hydrocortisone	10282201	1
Nachprüfung	Hydrocortisone	123456	1
Nachprüfung	Hydrocortisone	2082019-6	1
Noweda 28.10.2019	Hydrocortisone	18091531	1
Noweda 5,45 06.0...	Hydrocortisone	18324311	1
Noweda 5,45 14.04.2020	Hydrocortisone	183243002	1
Noweda Herford	Hydrocortisone	21001215006	1
Noweda/ Caesar&Loren...	Hydrocortisone	18324303	1
Noweda	Hydrocortisone	12104303	1
Noweda	Hydrocortisone	12167001	1
Noweda	Hydrocortisone	13155605	1
Noweda	Hydrocortisone	16004612	1
Noweda	Hydrocortisone	16095212	1
Noweda	Hydrocortisone	1611016-01	1
Noweda	Hydrocortisone	16255608	1
Noweda	Hydrocortisone	17090005	1
Noweda	Hydrocortisone	17119402	1
Noweda	Hydrocortisone	17256602	3
Noweda	Hydrocortisone	17256605	2
Noweda	Hydrocortisone	17351203	1
Noweda	Hydrocortisone	17351204	1
Noweda	Hydrocortisone	17351210	1
noweda	Hydrocortisone	18091506	1
Noweda	Hydrocortisone	183243002	2
Noweda	Hydrocortisone	18324301	1
Noweda	Hydrocortisone	18324308	1
Noweda	Hydrocortisone	18324311	1
Noweda	Hydrocortisone	192241005	1
Noweda	Hydrocortisone	192241008	1
Noweda	Hydrocortisone	20004116004	1
Noweda	Hydrocortisone	20004116005	2
Noweda	Hydrocortisone	20004116007	1
Noweda	Hydrocortisone	21001215003	4
Noweda	Hydrocortisone	22003779004	1
Noweda	Hydrocortisone	22003779006	2
NOWEDA	Hydrocortisone	22003779006	1
Otto Geilenkirchen	Hydrocortisone	21001215029	1
Pharmachem/ Anzag	Hydrocortisone	18091520	1
Pharmacia&Upjohn/ Phönix	Hydrocortisone	13155614	1
Phoenix	Hydrocortisone	13341504	1
Phoenix	Hydrocortisone	1509029-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Hydrocortisone	16095207	1
Phoenix	Hydrocortisone	1611016-01	1
Phoenix	Hydrocortisone	17119405	3
Phoenix	Hydrocortisone	17256605	1
Phoenix	Hydrocortisone	18091528	1
Phoenix	Hydrocortisone	18091531	1
Phoenix	Hydrocortisone	183243002	1
Phoenix	Hydrocortisone	18324301	1
Phoenix	Hydrocortisone	18324306	1
Phoenix	Hydrocortisone	18324311	1
phoenix	Hydrocortisone	192241008	1
Phoenix	Hydrocortisone	21001215005	1
Phoenix	Hydrocortisone	21001215029	1
Phoenix	Hydrocortisone	2101003-01	2
Phoenix	Hydrocortisone	3117	1
Phoenix	Hydrocortisone	3370	1
Phönix 15.7.2019	Hydrocortisone	18091520	1
Phönix Caesar u. Loretz	Hydrocortisone	13225507	1
Phönix Gotha	Hydrocortisone	12104309	1
Phönix Gotha	Hydrocortisone	13341502	1
Phönix Gotha	Hydrocortisone	15021107	1
Phönix Gotha	Hydrocortisone	15181004	1
Phönix Gotha	Hydrocortisone	18324307	1
Phönix, Caesar&Loret…	Hydrocortisone	183243003	1
phönix	Hydrocortisone		2
Phönix	Hydrocortisone	11119-N03	1
Phönix	Hydrocortisone	1204037-01	1
Phönix	Hydrocortisone	12167001	2
Phönix	Hydrocortisone	12167010	1
Phönix	Hydrocortisone	13341504	2
Phönix	Hydrocortisone	13341508	1
Phönix	Hydrocortisone	1408023-01	1
phönix	Hydrocortisone	14301306	1
Phönix	Hydrocortisone	15181005	1
phönix	Hydrocortisone	15181013	1
Phönix	Hydrocortisone	1611016-01	2
Phönix	Hydrocortisone	16110161-01	1
Phönix	Hydrocortisone	16272306	1
Phönix	Hydrocortisone	17119406	1
PHÖNIX	Hydrocortisone	17119410	1
Phönix	Hydrocortisone	17256602	1
Phönix	Hydrocortisone	17256603	1
Phönix	Hydrocortisone	17351206	2
Phönix	Hydrocortisone	17E10-B04-334858	1
Phönix	Hydrocortisone	1802009-01	3
Phönix	Hydrocortisone	18081508	1
Phönix	Hydrocortisone	18091505	1
Phönix	Hydrocortisone	1824302	1
Phönix	Hydrocortisone	183243006	1
Phönix	Hydrocortisone	18324302	1
Phönix	Hydrocortisone	18B21-B07-360920	1
Phönix	Hydrocortisone	1906033	1
Phönix	Hydrocortisone	1906033-01	3
PHÖNIX	Hydrocortisone	192241008	1
Phönix	Hydrocortisone	20004116002	1
Phönix	Hydrocortisone	20004116007	1
Phönix	Hydrocortisone	201073010	1
Phönix	Hydrocortisone	21001215005	3
Phönix	Hydrocortisone	21001215007	1
Phönix	Hydrocortisone	21001215032	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Hydrocortisone	2101003-01	2
Phönix	Hydrocortisone	22003779012	1
Phönix	Hydrocortisone	3181	1
Phönix	Hydrocortisone	Hy19	1
Röntgen	Hydrocortisone	17256605	1
Röntgen	Hydrocortisone	1906033-01	1
sana corp	Hydrocortisone	13069507	1
Sana	Hydrocortisone	18091524	3
Sanacorp	Hydrocortisone	1112030-01	1
Sanacorp	Hydrocortisone	13069509	1
Sanacorp	Hydrocortisone	13341509	1
Sanacorp	Hydrocortisone	14301307	1
Sanacorp	Hydrocortisone	14B04-B02	1
Sanacorp	Hydrocortisone	1509029-01	1
sanacorp	Hydrocortisone	15181012	1
sanacorp	Hydrocortisone	15181013	1
Sanacorp	Hydrocortisone	16004607	1
Sanacorp	Hydrocortisone	17256604	1
Sanacorp	Hydrocortisone	1802009-01	3
Sanacorp	Hydrocortisone	18091501	1
Sanacorp	Hydrocortisone	18091507	1
Sanacorp	Hydrocortisone	18091520	1
Sanacorp	Hydrocortisone	183243006	1
Sanacorp	Hydrocortisone	1906033-01	1
sanacorp	Hydrocortisone	192241008	1
Sanacorp	Hydrocortisone	192241008	3
Sanacorp	Hydrocortisone	20b17-b02-200514	1
Sanacorp	Hydrocortisone	21001215014	1
Sanacorp	Hydrocortisone	21001215023	2
Sanacorp	Hydrocortisone	22003779004	2
Sanacorp	Hydrocortisone	42/AKD6	1
Sanacorp	Hydrocortisone	Fagron	1
Sanacorp	Hydrocortisone	K05M20221003	1
Spangro 22.05.2014	Hydrocortisone	13341504	2
Spangro 23.1.2014	Hydrocortisone	13069510	1
Spangro_21.05.2019	Hydrocortisone	18091524	1
Tianjin JP / Gehe	Hydrocortisone	183243004	1
Tianjin/Noweda	Hydrocortisone	T3307	1
Tianjin/Noweda	Hydrocortisone	TA0075	1
Upjohn/Phönix	Hydrocortisone	1509029-01	1
VDL	Hydrocortisone	18091525	1
xxx	Hydrocortisone	911Q-01719	2

- 231 571 spectra from 1514 *Apo-Ident* customers from a total of 48 711 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hydrocortisone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hydrocortisone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	661	0	152 301
Type B	0	1119	0	200 965
Type C	0	4487	9	231 571

The substance/substance group *Hydrocortisone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4638 %)
Type C	100.0000 % (> 99.9007 %)	99.7998 % (> 99.7331 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21293	21899	7.22	116.60
21461	21899	8.00	117.12
21463	21899	3.34	117.05
21899	21899	0.00	117.25
22829	22838	7.67	119.75
22837	22838	5.18	117.60
22838	22838	0.00	119.73
22910	22910	0.00	120.10
22928	22910	5.74	122.00
24020	24020	0.00	119.55
25571	25571	0.00	122.58

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hydrocortisone acetate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20010-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hydrocortisone acetate; Hydrocortisoni acetas

Special notes

When selecting the *Hydrocortisone acetate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hydrocortisone acetate	7	16	594

Second-stage model

For differentiation of the substance/substance group *Hydrocortisone acetate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hydrocortisone acetate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	102.09	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hydrocortisone acetate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hydrocortisone acetate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hydrocortisone acetate	13291708	21462	60	20130926
Caelo	Hydrocortisone acetate	182780	24392	40	20181210*
Euro OTC	Hydrocortisone acetate	1209003-01	21295	40	20121108
Euro OTC	Hydrocortisone acetate	1209003-01	21295SI	45	20121108
Euro OTC	Hydrocortisone acetate	1508029	21889	60	20150902*
Euro OTC	Hydrocortisone acetate	1508029	21889SI	44	20150902*
Euro OTC	Hydrocortisone acetate	1604052	22564	40	20160525*
Fagron	Hydrocortisone acetate	15A30-B09-307090	22241	60	20150226
Fagron	Hydrocortisone acetate	18H07-B03-356259	24590	40	20180829

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 429 spectra of 9 reference samples from the substance/substance group *Hydrocortisone acetate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 533 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1296 spectra of 36 reference samples from the substance/substance group *Hydrocortisone - acetate*.

- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydrocortisone acetate	16238706	23115	40
Caelo	Hydrocortisone acetate	170862	23328	40
Caelo	Hydrocortisone acetate	21002415001	25924	40
Caelo	Hydrocortisone acetate	21003553	25992	40
Caelo	Hydrocortisone acetate	22002539	26363	40
Caelo	Hydrocortisone acetate	23001089	26853	40
Caelo	Hydrocortisone acetate	23003142	27133	40
Euro OTC	Hydrocortisone acetate	1706021	23559	40
Euro OTC	Hydrocortisone acetate	1805010	24130	40
Euro OTC	Hydrocortisone acetate	1907011	24789	40
Euro OTC	Hydrocortisone acetate	2004029	25331	40
Euro OTC	Hydrocortisone acetate	2205004	26212	40
Euro OTC	Hydrocortisone acetate	2306007	26883	40
Euro OTC	Hydrocortisone acetate	2406005	27349	40
Fagron	Hydrocortisone acetate	22A17-B07-216283	26138	40
Fagron	Hydrocortisone acetate	23E18-B03-229951	27266	40
Caelo	Hydrocortisone acetate	16238706	23115SI	20
Caelo	Hydrocortisone acetate	170862	23328SI	21
Caelo	Hydrocortisone acetate	182780	24392SI†	32
Caelo	Hydrocortisone acetate	21002415001	25924SI	40
Caelo	Hydrocortisone acetate	21003553	25992SI	35
Caelo	Hydrocortisone acetate	22002539	26363SI	40
Caelo	Hydrocortisone acetate	23001089	26853SI	40
Caelo	Hydrocortisone acetate	23003142	27133SI	30
Euro OTC	Hydrocortisone acetate	1604052	22564SI†	30
Euro OTC	Hydrocortisone acetate	1706021	23559SI	30
Euro OTC	Hydrocortisone acetate	1805010	24130SI	21
Euro OTC	Hydrocortisone acetate	1907011	24789SI	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Hydrocortisone acetate	2004029	25331SI	40
Euro OTC	Hydrocortisone acetate	2205004	26212SI	20
Euro OTC	Hydrocortisone acetate	2306007	26883SI	40
Euro OTC	Hydrocortisone acetate	2406005	27349SI	40
Fagron	Hydrocortisone acetate	15A30-B09-307090	22241SI[†]	24
Fagron	Hydrocortisone acetate	18H07-B03-356259	24590SI[†]	33
Fagron	Hydrocortisone acetate	22A17-B07-216283	26138SI	40
Fagron	Hydrocortisone acetate	23E18-B03-229951	27266SI	40

- 200 788 spectra from a total of 4025 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5588 spectra from 1259 *Apo-Ident* customers from 613 batches from the substance/substance group *Hydrocortisone acetate*.
- Among them are spectra of independent samples from 591 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Hydrocortisone acetate	14043902	1
	Hydrocortisone acetate	21002415010	1
	Hydrocortisone acetate	21002415011	1
	Hydrocortisone acetate	21002415013	2
	Hydrocortisone acetate	21002415014	1
	Hydrocortisone acetate	21002415015	1
	Hydrocortisone acetate	21003553006	1
	Hydrocortisone acetate	2100415014	1
	Hydrocortisone acetate	22002539002	11
	Hydrocortisone acetate	22002539003	2
	Hydrocortisone acetate	22002539004	7
	Hydrocortisone acetate	22002539008	7
	Hydrocortisone acetate	22002539009	13
	Hydrocortisone acetate	22002539010	14
	Hydrocortisone acetate	22002539013	17
	Hydrocortisone acetate	22002539014	8
	Hydrocortisone acetate	22002539015	17
	Hydrocortisone acetate	22002539016	1
	Hydrocortisone acetate	22002539018	6
	Hydrocortisone acetate	22002539019	10
	Hydrocortisone acetate	2200253904	2
	Hydrocortisone acetate	2202539004	1
	Hydrocortisone acetate	2205004-01	3
	Hydrocortisone acetate	22H11-B01-229287	2
	Hydrocortisone acetate	22K21-B02-225805	2
	Hydrocortisone acetate	23001089003	2
	Hydrocortisone acetate	23001089004	3

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Hydrocortisone acetate	23001089005	20
	Hydrocortisone acetate	23001089006	11
	Hydrocortisone acetate	23001089009	10
	Hydrocortisone acetate	23003142003	5
	Hydrocortisone acetate	2306007-01	2
	Hydrocortisone acetate	333961	1
	Hydrocortisone acetate	HD0125	1
AEP	Hydrocortisone acetate	18278005	1
AEP	Hydrocortisone acetate	18278020	4
AHD 07.03.2017 EK: 5,33	Hydrocortisone acetate	16004407	1
AHD/Euro	Hydrocortisone acetate	1706021-01	1
AHD/Euro	Hydrocortisone acetate	1805010-01	1
AHD	Hydrocortisone acetate	1205034-01	1
AHD	Hydrocortisone acetate	13291707	1
AHD	Hydrocortisone acetate	1706021-01	1
AHD	Hydrocortisone acetate	17219704	1
AHD	Hydrocortisone acetate	17219708	1
AHD	Hydrocortisone acetate	21002415004	1
AHD	Hydrocortisone acetate	22002539003	1
AHD	Hydrocortisone acetate	22002539009	1
AHD	Hydrocortisone acetate	22002539013	1
AHD	Hydrocortisone acetate	22002539018	1
AHD	Hydrocortisone acetate	23001089006	1
AHD;05,02,15; 12.48EUR	Hydrocortisone acetate	14144805	1
Alliance Healthcare	Hydrocortisone acetate	20004117001	2
Alliance Healthcare	Hydrocortisone acetate	21002415011	1
Alliance Healthcare	Hydrocortisone acetate	22002539010	1
Alliance/EurRho	Hydrocortisone acetate	1907011-02	1
Alliance/EurRho	Hydrocortisone acetate	2004029-01	2
Alliance	Hydrocortisone acetate	1604052-01	1
Alliance	Hydrocortisone acetate	2004029-02	1
Alliance	Hydrocortisone acetate	21002415014	1
Alliance	Hydrocortisone acetate	21003553007	2
Alliance	Hydrocortisone acetate	22002539014	1
Allianz Healthcare	Hydrocortisone acetate	18278005	1
Allianz Healthcare	Hydrocortisone acetate	18278021	1
Allianz	Hydrocortisone acetate	17219705	1
AMH Niemann/Sanacorp	Hydrocortisone acetate	17219705	1
Anzag 20.12.17 5.28	Hydrocortisone acetate	17219702	1
Anzag	Hydrocortisone acetate	1112031-02	1
Anzag	Hydrocortisone acetate	1209003-01	1
Anzag	Hydrocortisone acetate	16238708	1
Anzag	Hydrocortisone acetate	16238712	1
Anzag	Hydrocortisone acetate	16238713	1
Anzag	Hydrocortisone acetate	17086206	2
Anzag	Hydrocortisone acetate	17219702	2
Anzag	Hydrocortisone acetate	17219703	1
Anzag	Hydrocortisone acetate	18278021	2
Anzag	Hydrocortisone acetate	20004117001	1
Anzag	Hydrocortisone acetate	22002539013	1
Anzag	Hydrocortisone acetate	2205004-01	1
Apo-ident	Hydrocortisone acetate	1805010-01	1
Apo-ident	Hydrocortisone acetate	1907011-01	1
apomix	Hydrocortisone acetate	1404017-02	1
apomix	Hydrocortisone acetate	16095407	1
Bombastus	Hydrocortisone acetate	123Validierung	1
Bombastus	Hydrocortisone acetate	1505008-03	1
Bombastus	Hydrocortisone acetate	15356903	1
Bombastus	Hydrocortisone acetate	1604052-01	1
Bombastus	Hydrocortisone acetate	2712M01718	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caeelo	Hydrocortisone acetate	17086204	1
Caello/Anzag	Hydrocortisone acetate	15067003	1
Caelo	Hydrocortisone acetate		7
Caelo	Hydrocortisone acetate	10024150042	1
Caelo	Hydrocortisone acetate	10024150112	1
Caelo	Hydrocortisone acetate	10301904	1
Caelo	Hydrocortisone acetate	1061704	1
Caelo	Hydrocortisone acetate	11098604	1
Caelo	Hydrocortisone acetate	11098612	1
Caelo	Hydrocortisone acetate	11098615	1
Caelo	Hydrocortisone acetate	1112031-02	1
Caelo	Hydrocortisone acetate	11263902	1
Caelo	Hydrocortisone acetate	11263905	1
Caelo	Hydrocortisone acetate	11263913	1
Caelo	Hydrocortisone acetate	11263915	2
Caelo	Hydrocortisone acetate	11263916	1
Caelo	Hydrocortisone acetate	11263917	3
Caelo	Hydrocortisone acetate	1130317	1
Caelo	Hydrocortisone acetate	118107-3	1
Caelo	Hydrocortisone acetate	12008402	2
Caelo	Hydrocortisone acetate	12008405	4
Caelo	Hydrocortisone acetate	12021502	1
Caelo	Hydrocortisone acetate	1205034-01	3
Caelo	Hydrocortisone acetate	1209003-01	6
Caelo	Hydrocortisone acetate	12121801	1
Caelo	Hydrocortisone acetate	1213M-01718	1
Caelo	Hydrocortisone acetate	12182402	10
Caelo	Hydrocortisone acetate	12182403	5
Caelo	Hydrocortisone acetate	12182404	19
Caelo	Hydrocortisone acetate	12182405	17
Caelo	Hydrocortisone acetate	12182408	2
Caelo	Hydrocortisone acetate	12183403	1
Caelo	Hydrocortisone acetate	12330102	8
Caelo	Hydrocortisone acetate	12330103	8
Caelo	Hydrocortisone acetate	12330104	9
Caelo	Hydrocortisone acetate	12330105	3
Caelo	Hydrocortisone acetate	12330106	4
Caelo	Hydrocortisone acetate	12330107	8
Caelo	Hydrocortisone acetate	12330108	15
Caelo	Hydrocortisone acetate	12330110	2
Caelo	Hydrocortisone acetate	12330111	3
Caelo	Hydrocortisone acetate	12330111-3507411061	1
Caelo	Hydrocortisone acetate	12330112	13
Caelo	Hydrocortisone acetate	12330113	1
Caelo	Hydrocortisone acetate	12330114	1
Caelo	Hydrocortisone acetate	12330116	10
Caelo	Hydrocortisone acetate	13155302	8
Caelo	Hydrocortisone acetate	13155303	9
Caelo	Hydrocortisone acetate	13155304	5
Caelo	Hydrocortisone acetate	13155306	5
Caelo	Hydrocortisone acetate	13155307	2
Caelo	Hydrocortisone acetate	13155308	8
Caelo	Hydrocortisone acetate	131553080	1
Caelo	Hydrocortisone acetate	13291701	1
Caelo	Hydrocortisone acetate	13291704	4
Caelo	Hydrocortisone acetate	13291705	4
Caelo	Hydrocortisone acetate	13291706	10
Caelo	Hydrocortisone acetate	13291707	14
Caelo	Hydrocortisone acetate	13291708	7
Caelo	Hydrocortisone acetate	13291709	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hydrocortisone acetate	13291711	7
Caelo	Hydrocortisone acetate	1391704	1
Caelo	Hydrocortisone acetate	1391706	1
Caelo	Hydrocortisone acetate	13G09-N08	2
Caelo	Hydrocortisone acetate	1403903	1
Caelo	Hydrocortisone acetate	14043901	11
Caelo	Hydrocortisone acetate	14043902	10
Caelo	Hydrocortisone acetate	14043903	12
Caelo	Hydrocortisone acetate	14043904	14
Caelo	Hydrocortisone acetate	14043905	11
Caelo	Hydrocortisone acetate	14043906	9
Caelo	Hydrocortisone acetate	14043907	14
Caelo	Hydrocortisone acetate	14043908	1
Caelo	Hydrocortisone acetate	1406211718	1
Caelo	Hydrocortisone acetate	14144802	1
Caelo	Hydrocortisone acetate	14144803	9
Caelo	Hydrocortisone acetate	14144804	6
Caelo	Hydrocortisone acetate	14144805	21
Caelo	Hydrocortisone acetate	14144806	15
Caelo	Hydrocortisone acetate	14144807	6
Caelo	Hydrocortisone acetate	1430102	1
Caelo	Hydrocortisone acetate	1430140	1
Caelo	Hydrocortisone acetate	14301401	15
Caelo	Hydrocortisone acetate	14301402	8
Caelo	Hydrocortisone acetate	14301403	6
Caelo	Hydrocortisone acetate	14301404	7
Caelo	Hydrocortisone acetate	14301405	24
Caelo	Hydrocortisone acetate	14301406	18
Caelo	Hydrocortisone acetate	14301407	17
Caelo	Hydrocortisone acetate	14301408	8
Caelo	Hydrocortisone acetate	14I16-B01-300292	1
Caelo	Hydrocortisone acetate	1501035	1
Caelo	Hydrocortisone acetate	1505008-01	6
Caelo	Hydrocortisone acetate	15061006	1
Caelo	Hydrocortisone acetate	15061207	1
Caelo	Hydrocortisone acetate	15067003	13
Caelo	Hydrocortisone acetate	15067004	26
Caelo	Hydrocortisone acetate	15067005	18
Caelo	Hydrocortisone acetate	15067006	13
Caelo	Hydrocortisone acetate	15067010	3
Caelo	Hydrocortisone acetate	15067011	8
Caelo	Hydrocortisone acetate	15067013	11
Caelo	Hydrocortisone acetate	1508029-01	4
Caelo	Hydrocortisone acetate	15216204	3
Caelo	Hydrocortisone acetate	15356901	17
Caelo	Hydrocortisone acetate	15356902	20
Caelo	Hydrocortisone acetate	15356903	23
Caelo	Hydrocortisone acetate	15356904	8
Caelo	Hydrocortisone acetate	1536902	1
Caelo	Hydrocortisone acetate	15A07-B03-306545	1
Caelo	Hydrocortisone acetate	15H24_B01-316480	1
Caelo	Hydrocortisone acetate	15H24-B01-314236	2
Caelo	Hydrocortisone acetate	1600406	1
Caelo	Hydrocortisone acetate	160044003	1
Caelo	Hydrocortisone acetate	16004402	19
Caelo	Hydrocortisone acetate	16004403	9
Caelo	Hydrocortisone acetate	16004404	1
Caelo	Hydrocortisone acetate	16004405	13
Caelo	Hydrocortisone acetate	16004406	27
Caelo	Hydrocortisone acetate	16004407	23

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hydrocortisone acetate	16004408	22
Caelo	Hydrocortisone acetate	160044402	1
Caelo	Hydrocortisone acetate	1604052	1
Caelo	Hydrocortisone acetate	1604052-01	6
Caelo	Hydrocortisone acetate	1605410	1
Caelo	Hydrocortisone acetate	160629HA	1
Caelo	Hydrocortisone acetate	16095402	1
Caelo	Hydrocortisone acetate	16095404	33
Caelo	Hydrocortisone acetate	16095405	22
Caelo	Hydrocortisone acetate	16095406	26
Caelo	Hydrocortisone acetate	16095407	37
Caelo	Hydrocortisone acetate	16095408	4
Caelo	Hydrocortisone acetate	16095410	7
Caelo	Hydrocortisone acetate	1623708	1
Caelo	Hydrocortisone acetate	16238704	11
Caelo	Hydrocortisone acetate	16238705	3
Caelo	Hydrocortisone acetate	16238706	34
Caelo	Hydrocortisone acetate	16238706-12517/2	1
Caelo	Hydrocortisone acetate	16238707	15
Caelo	Hydrocortisone acetate	16238708	25
Caelo	Hydrocortisone acetate	16238708-200417/1	1
Caelo	Hydrocortisone acetate	16238709	8
Caelo	Hydrocortisone acetate	16238710	23
Caelo	Hydrocortisone acetate	16238712	25
Caelo	Hydrocortisone acetate	16238713	8
Caelo	Hydrocortisone acetate	16238713-20170818Ma2	1
Caelo	Hydrocortisone acetate	16238714	12
Caelo	Hydrocortisone acetate	1623888704	1
Caelo	Hydrocortisone acetate	163163055402	1
Caelo	Hydrocortisone acetate	166004407	1
Caelo	Hydrocortisone acetate	16C15-B04-321459	1
Caelo	Hydrocortisone acetate	17011402	1
Caelo	Hydrocortisone acetate	17053185	1
Caelo	Hydrocortisone acetate	170602101	1
Caelo	Hydrocortisone acetate	1706021-01	11
Caelo	Hydrocortisone acetate	170804HA/1604052-01	1
Caelo	Hydrocortisone acetate	170856206	1
Caelo	Hydrocortisone acetate	17086202	1
Caelo	Hydrocortisone acetate	170862024	1
Caelo	Hydrocortisone acetate	17086203	18
Caelo	Hydrocortisone acetate	17086204	27
Caelo	Hydrocortisone acetate	17086205	28
Caelo	Hydrocortisone acetate	17086205-20170818Ma3	1
Caelo	Hydrocortisone acetate	17086206	11
Caelo	Hydrocortisone acetate	17086207	4
Caelo	Hydrocortisone acetate	17086209	2
Caelo	Hydrocortisone acetate	17086211	10
Caelo	Hydrocortisone acetate	17086212	3
Caelo	Hydrocortisone acetate	17086221	1
Caelo	Hydrocortisone acetate	171106HA/17086204	1
Caelo	Hydrocortisone acetate	17142802	1
Caelo	Hydrocortisone acetate	1721905	1
Caelo	Hydrocortisone acetate	17219702	21
Caelo	Hydrocortisone acetate	17219703	26
Caelo	Hydrocortisone acetate	17219704	26
Caelo	Hydrocortisone acetate	17219705	65
Caelo	Hydrocortisone acetate	172197050	1
Caelo	Hydrocortisone acetate	172197055662	1
Caelo	Hydrocortisone acetate	17219706	31
Caelo	Hydrocortisone acetate	17219707	49

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hydrocortisone acetate	17219708	47
Caelo	Hydrocortisone acetate	172197085556	1
Caelo	Hydrocortisone acetate	17219709	8
Caelo	Hydrocortisone acetate	17219710	2
Caelo	Hydrocortisone acetate	17219713	4
Caelo	Hydrocortisone acetate	17219714	1
Caelo	Hydrocortisone acetate	17358402	1
Caelo	Hydrocortisone acetate	17358403	9
Caelo	Hydrocortisone acetate	17358404	1
Caelo	Hydrocortisone acetate	17L19-B04-348983	1
Caelo	Hydrocortisone acetate	18011304	1
Caelo	Hydrocortisone acetate	180219HA/17219707	1
Caelo	Hydrocortisone acetate	1805010-01	1
Caelo	Hydrocortisone acetate	181115181	1
Caelo	Hydrocortisone acetate	18121710	1
Caelo	Hydrocortisone acetate	18142802	16
Caelo	Hydrocortisone acetate	18142803	13
Caelo	Hydrocortisone acetate	18142804	39
Caelo	Hydrocortisone acetate	18142805	45
Caelo	Hydrocortisone acetate	18142805-H20181115Ma	1
Caelo	Hydrocortisone acetate	18142806	42
Caelo	Hydrocortisone acetate	18142807	26
Caelo	Hydrocortisone acetate	18142808	21
Caelo	Hydrocortisone acetate	181428087	1
Caelo	Hydrocortisone acetate	18142809	21
Caelo	Hydrocortisone acetate	18142810	2
Caelo	Hydrocortisone acetate	18142811	18
Caelo	Hydrocortisone acetate	18142812	23
Caelo	Hydrocortisone acetate	18142814	1
Caelo	Hydrocortisone acetate	18142815	18
Caelo	Hydrocortisone acetate	18142904	1
Caelo	Hydrocortisone acetate	181442805	1
Caelo	Hydrocortisone acetate	1827006	1
Caelo	Hydrocortisone acetate	1827015	1
Caelo	Hydrocortisone acetate	18278003	22
Caelo	Hydrocortisone acetate	18278004	39
Caelo	Hydrocortisone acetate	18278005	59
Caelo	Hydrocortisone acetate	18278006	29
Caelo	Hydrocortisone acetate	18278007	24
Caelo	Hydrocortisone acetate	18278008	23
Caelo	Hydrocortisone acetate	18278010	36
Caelo	Hydrocortisone acetate	18278011	1
Caelo	Hydrocortisone acetate	18278014	23
Caelo	Hydrocortisone acetate	18278015	33
Caelo	Hydrocortisone acetate	18278016	30
Caelo	Hydrocortisone acetate	18278017	5
Caelo	Hydrocortisone acetate	18278018	20
Caelo	Hydrocortisone acetate	18278019	22
Caelo	Hydrocortisone acetate	18278020	24
Caelo	Hydrocortisone acetate	18278021	22
Caelo	Hydrocortisone acetate	18278021ma	1
Caelo	Hydrocortisone acetate	1828007	1
Caelo	Hydrocortisone acetate	1828014	1
Caelo	Hydrocortisone acetate	187278005	1
Caelo	Hydrocortisone acetate	18H07-B03-357240	2
Caelo	Hydrocortisone acetate	190372703	1
Caelo	Hydrocortisone acetate	1907011-02	1
Caelo	Hydrocortisone acetate	190910209	1
Caelo	Hydrocortisone acetate	1913807	1
Caelo	Hydrocortisone acetate	191383001	10

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hydrocortisone acetate	191383004	19
Caelo	Hydrocortisone acetate	19138301	24
Caelo	Hydrocortisone acetate	19138302	18
Caelo	Hydrocortisone acetate	19138303	1
Caelo	Hydrocortisone acetate	19138304	29
Caelo	Hydrocortisone acetate	19138305	29
Caelo	Hydrocortisone acetate	19138306	1
Caelo	Hydrocortisone acetate	19138307	43
Caelo	Hydrocortisone acetate	19138308	8
Caelo	Hydrocortisone acetate	1918304	1
Caelo	Hydrocortisone acetate	192241005	2
Caelo	Hydrocortisone acetate	192241008	1
Caelo	Hydrocortisone acetate	1938305	1
Caelo	Hydrocortisone acetate	19j10-f04-366276	1
Caelo	Hydrocortisone acetate	19J10-F04-366276	1
Caelo	Hydrocortisone acetate	200000978004	1
Caelo	Hydrocortisone acetate	200000978007	1
Caelo	Hydrocortisone acetate	200004117001	1
Caelo	Hydrocortisone acetate	2000078008	1
Caelo	Hydrocortisone acetate	20000977002	13
Caelo	Hydrocortisone acetate	20000978003	1
Caelo	Hydrocortisone acetate	20000978004	34
Caelo	Hydrocortisone acetate	20000978005	28
Caelo	Hydrocortisone acetate	20000978006	31
Caelo	Hydrocortisone acetate	20000978007	23
Caelo	Hydrocortisone acetate	20000978008	21
Caelo	Hydrocortisone acetate	20000978009	12
Caelo	Hydrocortisone acetate	20000978010	8
Caelo	Hydrocortisone acetate	2000097808	1
Caelo	Hydrocortisone acetate	200009978005	1
Caelo	Hydrocortisone acetate	20001708003	1
Caelo	Hydrocortisone acetate	200041117006	1
Caelo	Hydrocortisone acetate	200041147001	1
Caelo	Hydrocortisone acetate	20004117001	65
Caelo	Hydrocortisone acetate	20004117004	15
Caelo	Hydrocortisone acetate	20004117005	4
Caelo	Hydrocortisone acetate	20004117006	18
Caelo	Hydrocortisone acetate	20004117007	3
Caelo	Hydrocortisone acetate	2000411701	1
Caelo	Hydrocortisone acetate	200041176	1
Caelo	Hydrocortisone acetate	2000417001	2
Caelo	Hydrocortisone acetate	20004278002	22
Caelo	Hydrocortisone acetate	20004278003	30
Caelo	Hydrocortisone acetate	20004278004	54
Caelo	Hydrocortisone acetate	20004278005	16
Caelo	Hydrocortisone acetate	20004278006	8
Caelo	Hydrocortisone acetate	20004278008	13
Caelo	Hydrocortisone acetate	20004278009	8
Caelo	Hydrocortisone acetate	2000427806	1
Caelo	Hydrocortisone acetate	2000977002	1
Caelo	Hydrocortisone acetate	2000978008	1
Caelo	Hydrocortisone acetate	2004029-01	2
Caelo	Hydrocortisone acetate	2004117001	2
Caelo	Hydrocortisone acetate	2004117006	1
Caelo	Hydrocortisone acetate	2004117007	2
Caelo	Hydrocortisone acetate	2004278005	1
Caelo	Hydrocortisone acetate	2004278008	1
Caelo	Hydrocortisone acetate	200660707	1
Caelo	Hydrocortisone acetate	20160727Ma2	1
Caelo	Hydrocortisone acetate	2021803	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hydrocortisone acetate	2061401	1
Caelo	Hydrocortisone acetate	2100215013	1
Caelo	Hydrocortisone acetate	210024150002	1
Caelo	Hydrocortisone acetate	21002415001	35
Caelo	Hydrocortisone acetate	21002415002	27
Caelo	Hydrocortisone acetate	21002415004	31
Caelo	Hydrocortisone acetate	21002415005	7
Caelo	Hydrocortisone acetate	21002415006	21
Caelo	Hydrocortisone acetate	21002415007	1
Caelo	Hydrocortisone acetate	21002415008	6
Caelo	Hydrocortisone acetate	21002415009	18
Caelo	Hydrocortisone acetate	21002415010	12
Caelo	Hydrocortisone acetate	21002415011	35
Caelo	Hydrocortisone acetate	21002415012	13
Caelo	Hydrocortisone acetate	21002415014	15
Caelo	Hydrocortisone acetate	21002415015	3
Caelo	Hydrocortisone acetate	2100245011	1
Caelo	Hydrocortisone acetate	21003093011	1
Caelo	Hydrocortisone acetate	2100355	1
Caelo	Hydrocortisone acetate	210035530004	1
Caelo	Hydrocortisone acetate	21003553002	1
Caelo	Hydrocortisone acetate	21003553003	4
Caelo	Hydrocortisone acetate	21003553004	16
Caelo	Hydrocortisone acetate	21003553005	17
Caelo	Hydrocortisone acetate	21003553006	11
Caelo	Hydrocortisone acetate	21003553007	11
Caelo	Hydrocortisone acetate	21003553009	4
Caelo	Hydrocortisone acetate	21003553010	3
Caelo	Hydrocortisone acetate	2100415004	1
Caelo	Hydrocortisone acetate	2100415009	1
Caelo	Hydrocortisone acetate	2200253008	1
Caelo	Hydrocortisone acetate	22002539	1
Caelo	Hydrocortisone acetate	22002539002	10
Caelo	Hydrocortisone acetate	22002539003	9
Caelo	Hydrocortisone acetate	22002539004	2
Caelo	Hydrocortisone acetate	22002539005	3
Caelo	Hydrocortisone acetate	22002539008	6
Caelo	Hydrocortisone acetate	22002539009	1
Caelo	Hydrocortisone acetate	22002539010	6
Caelo	Hydrocortisone acetate	22002539013	1
Caelo	Hydrocortisone acetate	22002539014	2
Caelo	Hydrocortisone acetate	22002539015	4
Caelo	Hydrocortisone acetate	22002539018	1
Caelo	Hydrocortisone acetate	22002539019	2
Caelo	Hydrocortisone acetate	2202539003	1
Caelo	Hydrocortisone acetate	2202539004	1
Caelo	Hydrocortisone acetate	2202539008	1
Caelo	Hydrocortisone acetate	23001089004	1
Caelo	Hydrocortisone acetate	25(1805010-01)	1
Caelo	Hydrocortisone acetate	25101201	1
Caelo	Hydrocortisone acetate	2612M01718	1
Caelo	Hydrocortisone acetate	27091307	1
Caelo	Hydrocortisone acetate	27091403	1
Caelo	Hydrocortisone acetate	2734	1
Caelo	Hydrocortisone acetate	28071508	1
Caelo	Hydrocortisone acetate	301115	1
Caelo	Hydrocortisone acetate	3110491	1
Caelo	Hydrocortisone acetate	3110516	1
Caelo	Hydrocortisone acetate	3434	1
Caelo	Hydrocortisone acetate	418M-01718	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hydrocortisone acetate	6071801	1
Caelo	Hydrocortisone acetate	6101707	1
Caelo	Hydrocortisone acetate	7051303	1
Caelo	Hydrocortisone acetate	7082003	1
Caelo	Hydrocortisone acetate	7086205	1
Caelo	Hydrocortisone acetate	84280411	1
Caelo	Hydrocortisone acetate	978004	1
Caelo	Hydrocortisone acetate	Caelo	2
Caelo	Hydrocortisone acetate	Caelo/20004117005	1
Caelo	Hydrocortisone acetate	Hydc01122022	1
Caelo	Hydrocortisone acetate	NCEHAC161003	1
Caelo	Hydrocortisone acetate	test	1
Caeol/Noweda	Hydrocortisone acetate	19138307	1
Caeol/Phoenix	Hydrocortisone acetate	16004402	1
Caeol/Phönix	Hydrocortisone acetate	17219708	1
Caeolo/Noweda	Hydrocortisone acetate	13155303	1
Caeolo/Spangro	Hydrocortisone acetate	20000978004	1
Caesar & Lorenz GmbH	Hydrocortisone acetate	18278016	1
Caesar & Lorenz GmbH	Hydrocortisone acetate	19138305	1
Caesar & Lorenz GmbH	Hydrocortisone acetate	20000978007	1
Caesar & Loretz /Alliance	Hydrocortisone acetate	21002415010	2
Caesar & Loretz GmbH…	Hydrocortisone acetate	14144806	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	19138308	4
Caesar & Loretz GmbH…	Hydrocortisone acetate	20004117005	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	21002415006	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	21002415008	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	21002415013	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	18278014	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	21003553006	2
Caesar & Loretz GmbH…	Hydrocortisone acetate	18278020	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	20004278003	2
Caesar & Loretz GmbH, Now	Hydrocortisone acetate	22002539002	1
Caesar & Loretz GmbH/ AEP	Hydrocortisone acetate	19138305	1
Caesar & Loretz GmbH/ AHD	Hydrocortisone acetate	20000978010	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	21002415011	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	20004117006	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	20004278004	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	21003553006	2
Caesar & Loretz GmbH…	Hydrocortisone acetate	21003553009	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	21002415011	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	21003553004	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	18278004	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	20004278004	2
Caesar & Loretz GmbH…	Hydrocortisone acetate	20004278006	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	21002415011	3
Caesar & Loretz GmbH…	Hydrocortisone acetate	20004117001	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	21002415004	1
Caesar & Loretz GmbH/AEP	Hydrocortisone acetate	18278014	1
Caesar & Loretz GmbH/AEP	Hydrocortisone acetate	21002415001	1
Caesar & Loretz GmbH/AHD	Hydrocortisone acetate	20004278003	1
Caesar & Loretz GmbH/AHD	Hydrocortisone acetate	21002415001	1
Caesar & Loretz GmbH/AHD	Hydrocortisone acetate	21002415011	2
Caesar & Loretz GmbH/AHD	Hydrocortisone acetate	21002415014	2
Caesar & Loretz GmbH/AHD	Hydrocortisone acetate	22002539004	3
Caesar & Loretz GmbH/all	Hydrocortisone acetate	20000978005	1
Caesar & Loretz GmbH/Alli	Hydrocortisone acetate	20000978004	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	191383001	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	19138307	1
Caesar & Loretz GmbH…	Hydrocortisone acetate	21002415006	2
Caesar & Loretz GmbH…	Hydrocortisone acetate	19138304	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Hydrocortisone acetate	20004117001	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	20000978007	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	20004278004	1
Caesar & Loretz GmbH/G	Hydrocortisone acetate	20000978009	1
Caesar & Loretz GmbH/G	Hydrocortisone acetate	21002415001	1
Caesar & Loretz GmbH/Gehe	Hydrocortisone acetate	20000978006	1
Caesar & Loretz GmbH/Gehe	Hydrocortisone acetate	20004117001	1
Caesar & Loretz GmbH/GEHE	Hydrocortisone acetate	20004117001	1
Caesar & Loretz GmbH/Gehe	Hydrocortisone acetate	20004117006	1
Caesar & Loretz GmbH/Gehe	Hydrocortisone acetate	20004117007	1
Caesar & Loretz GmbH/Gehe	Hydrocortisone acetate	20004278004	3
Caesar & Loretz GmbH/Gehe	Hydrocortisone acetate	21002415001	1
Caesar & Loretz GmbH/Gehe	Hydrocortisone acetate	21002415014	1
Caesar & Loretz GmbH/Gehe	Hydrocortisone acetate	23001089005	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	20000977002	2
Caesar & Loretz GmbH...	Hydrocortisone acetate	20004117004	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	20004278002	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415014	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21003553006	2
Caesar & Loretz GmbH...	Hydrocortisone acetate	22002539004	1
Caesar & Loretz GmbH/GEJE	Hydrocortisone acetate	19138302	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	20000978005	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415002	3
Caesar & Loretz GmbH...	Hydrocortisone acetate	18278014	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	18278021	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	20000977002	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	20000978006	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415006	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415011	1
Caesar & Loretz GmbH/K	Hydrocortisone acetate	18278015	1
Caesar & Loretz GmbH/K	Hydrocortisone acetate	19138301	1
Caesar & Loretz GmbH/K	Hydrocortisone acetate	20004278003	1
Caesar & Loretz GmbH/Kehr	Hydrocortisone acetate	18278016	1
Caesar & Loretz GmbH/Kehr	Hydrocortisone acetate	191383001	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	20000978009	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	20004278003	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415001	1
Caesar & Loretz GmbH/Now	Hydrocortisone acetate	20004278006	2
Caesar & Loretz GmbH...	Hydrocortisone acetate	18278017	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415001	2
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415002	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415006	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415014	3
Caesar & Loretz GmbH...	Hydrocortisone acetate	21003553009	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	191383004	2
Caesar & Loretz GmbH...	Hydrocortisone acetate	191383001	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	20004117005	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	20004278004	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415004	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415011	4
Caesar & Loretz GmbH...	Hydrocortisone acetate	18142806	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	18278005	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	191383004	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	19138301	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	19138304	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	20000978006	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	20004278004	2
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415002	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415006	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415010	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415014	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21003553006	2
Caesar & Loretz GmbH...	Hydrocortisone acetate	22002539004	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	22002539005	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	22002539013	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	19138305	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	19138307	3
Caesar & Loretz GmbH...	Hydrocortisone acetate	20000978005	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	20000978006	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	20000978007	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	20004117001	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415002	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415004	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415008	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21002415010	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21003553004	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	21003553009	1
Caesar & Loretz GmbH...	Hydrocortisone acetate	22002539003	1
Caesar & Loretz GmbH	Hydrocortisone acetate		1
Caesar & Loretz GmbH	Hydrocortisone acetate	12182405	1
Caesar & Loretz GmbH	Hydrocortisone acetate	15067004	1
Caesar & Loretz GmbH	Hydrocortisone acetate	16004402	1
Caesar & Loretz GmbH	Hydrocortisone acetate	16004408	1
Caesar & Loretz GmbH	Hydrocortisone acetate	16095405	1
Caesar & Loretz GmbH	Hydrocortisone acetate	16095406	2
Caesar & Loretz GmbH	Hydrocortisone acetate	16095407	2
Caesar & Loretz GmbH	Hydrocortisone acetate	17219706	1
Caesar & Loretz GmbH	Hydrocortisone acetate	17219708	1
Caesar & Loretz GmbH	Hydrocortisone acetate	18142804	3
Caesar & Loretz GmbH	Hydrocortisone acetate	18142815	3
Caesar & Loretz GmbH	Hydrocortisone acetate	182778014	1
Caesar & Loretz GmbH	Hydrocortisone acetate	18278003	10
Caesar & Loretz GmbH	Hydrocortisone acetate	18278004	9
Caesar & Loretz GmbH	Hydrocortisone acetate	18278005	11
Caesar & Loretz GmbH	Hydrocortisone acetate	18278006	3
Caesar & Loretz GmbH	Hydrocortisone acetate	18278007	3
Caesar & Loretz GmbH	Hydrocortisone acetate	18278008	3
Caesar & Loretz GmbH	Hydrocortisone acetate	18278010	10
Caesar & Loretz GmbH	Hydrocortisone acetate	18278014	9
Caesar & Loretz GmbH	Hydrocortisone acetate	18278015	11
Caesar & Loretz GmbH	Hydrocortisone acetate	18278016	10
Caesar & Loretz GmbH	Hydrocortisone acetate	18278018	10
Caesar & Loretz GmbH	Hydrocortisone acetate	18278019	5
Caesar & Loretz GmbH	Hydrocortisone acetate	18278020	5
Caesar & Loretz GmbH	Hydrocortisone acetate	18278021	7
Caesar & Loretz GmbH	Hydrocortisone acetate	191383001	3
Caesar & Loretz GmbH	Hydrocortisone acetate	191383004	5
Caesar & Loretz GmbH	Hydrocortisone acetate	19138301	3
Caesar & Loretz GmbH	Hydrocortisone acetate	19138302	4
Caesar & Loretz GmbH	Hydrocortisone acetate	19138303	1
Caesar & Loretz GmbH	Hydrocortisone acetate	19138304	9
Caesar & Loretz GmbH	Hydrocortisone acetate	19138305	8
Caesar & Loretz GmbH	Hydrocortisone acetate	19138307	11
Caesar & Loretz GmbH	Hydrocortisone acetate	19138308	2
Caesar & Loretz GmbH	Hydrocortisone acetate	19A24	1
Caesar & Loretz GmbH	Hydrocortisone acetate	20000977002	1
Caesar & Loretz GmbH	Hydrocortisone acetate	20000978004	10
Caesar & Loretz GmbH	Hydrocortisone acetate	20000978005	9
Caesar & Loretz GmbH	Hydrocortisone acetate	20000978006	8
Caesar & Loretz GmbH	Hydrocortisone acetate	20000978007	12

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Hydrocortisone acetate	20000978008	5
Caesar & Loretz GmbH	Hydrocortisone acetate	20000978009	4
Caesar & Loretz GmbH	Hydrocortisone acetate	20000978010	4
Caesar & Loretz GmbH	Hydrocortisone acetate	20004117001	25
Caesar & Loretz GmbH	Hydrocortisone acetate	20004117004	6
Caesar & Loretz GmbH	Hydrocortisone acetate	20004117005	1
Caesar & Loretz GmbH	Hydrocortisone acetate	20004117006	5
Caesar & Loretz GmbH	Hydrocortisone acetate	20004117007	5
Caesar & Loretz GmbH	Hydrocortisone acetate	20004278002	9
Caesar & Loretz GmbH	Hydrocortisone acetate	20004278003	15
Caesar & Loretz GmbH	Hydrocortisone acetate	20004278004	15
Caesar & Loretz GmbH	Hydrocortisone acetate	20004278005	2
Caesar & Loretz GmbH	Hydrocortisone acetate	20004278006	9
Caesar & Loretz GmbH	Hydrocortisone acetate	20004278008	1
Caesar & Loretz GmbH	Hydrocortisone acetate	20004278009	1
Caesar & Loretz GmbH	Hydrocortisone acetate	21002415001	16
Caesar & Loretz GmbH	Hydrocortisone acetate	21002415002	10
Caesar & Loretz GmbH	Hydrocortisone acetate	21002415004	4
Caesar & Loretz GmbH	Hydrocortisone acetate	21002415005	6
Caesar & Loretz GmbH	Hydrocortisone acetate	21002415006	7
Caesar & Loretz GmbH	Hydrocortisone acetate	21002415008	3
Caesar & Loretz GmbH	Hydrocortisone acetate	21002415009	2
Caesar & Loretz GmbH	Hydrocortisone acetate	21002415010	10
Caesar & Loretz GmbH	Hydrocortisone acetate	21002415011	14
Caesar & Loretz GmbH	Hydrocortisone acetate	21002415012	7
Caesar & Loretz GmbH	Hydrocortisone acetate	21002415014	1
Caesar & Loretz GmbH	Hydrocortisone acetate	21003553002	1
Caesar & Loretz GmbH	Hydrocortisone acetate	21003553004	2
Caesar & Loretz GmbH	Hydrocortisone acetate	21003553005	6
Caesar & Loretz GmbH	Hydrocortisone acetate	21003553006	7
Caesar & Loretz GmbH	Hydrocortisone acetate	21003553007	6
Caesar & Loretz GmbH	Hydrocortisone acetate	21003553009	4
Caesar & Loretz GmbH	Hydrocortisone acetate	21003553010	4
Caesar & Loretz GmbH	Hydrocortisone acetate	22002539002	6
Caesar & Loretz GmbH	Hydrocortisone acetate	22002539003	5
Caesar & Loretz GmbH	Hydrocortisone acetate	22002539004	3
Caesar & Loretz GmbH	Hydrocortisone acetate	22002539008	6
Caesar & Loretz GmbH	Hydrocortisone acetate	22002539019	2
Caesar & Loretz GmbH	Hydrocortisone acetate	23001089005	1
Caesar & Loretz GmbHAnzag	Hydrocortisone acetate	18278019	1
Caesar & Loretz Hild…	Hydrocortisone acetate	20000978004	1
Caesar & Loretz Hilden	Hydrocortisone acetate	18278005	1
Caesar & Loretz Hilden	Hydrocortisone acetate	19138307	1
Caesar & Loretz Hilden	Hydrocortisone acetate	20004278005	1
Caesar & Loretz/AHD	Hydrocortisone acetate	17219706	1
Caesar & Loretz/Geil…	Hydrocortisone acetate	20000978008	1
Caesar & Loretz/Geil…	Hydrocortisone acetate	20004278004	2
Caesar & Loretz	Hydrocortisone acetate	16095404	1
Caesar & Loretz	Hydrocortisone acetate	17086203	1
Caesar & Loretz	Hydrocortisone acetate	18142815	2
Caesar / Gehe	Hydrocortisone acetate	15067003	1
Caesar u Loretz	Hydrocortisone acetate	15067003	1
Caesar und Loretz GmbH	Hydrocortisone acetate	18278020	1
Caesar&Loretz GmbH,P…	Hydrocortisone acetate	16238708	1
Caesar&Loretz GmbH/AHD	Hydrocortisone acetate	15356903	1
Caesar&Loretz GmbH/Anzag	Hydrocortisone acetate	14301405	2
Caesar&Loretz GmbH	Hydrocortisone acetate	21002415002	1
Caesar&loretz,Phoenix	Hydrocortisone acetate	12182405	1
Caesar&loretz,Phoenix	Hydrocortisone acetate	12330103	1
caesar&loretz,PHönix…	Hydrocortisone acetate	15067003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar&LoretzGmbH, P...	Hydrocortisone acetate	18278006	1
Caesar/Gehe	Hydrocortisone acetate	20000978005	1
caesar	Hydrocortisone acetate	14301402	1
Caolo	Hydrocortisone acetate	17219707	2
Carli/ Phoenix	Hydrocortisone acetate	20004117004	1
Cealo / Noweda	Hydrocortisone acetate	13291707	1
Cealo, GEHE	Hydrocortisone acetate	20004278002	2
Cealo/ Anzag	Hydrocortisone acetate	16238712	1
Cealo/ Anzag	Hydrocortisone acetate	17219702	1
Cealo/ Noweda	Hydrocortisone acetate	20000978008	1
Cealo/Gehe	Hydrocortisone acetate	16095410	2
Cealo/Noweda	Hydrocortisone acetate	18278016	2
Cealo/Sanacorp	Hydrocortisone acetate	20000978009	1
Cealo	Hydrocortisone acetate	1706021-01	1
Eplus	Hydrocortisone acetate	17219708	1
EuRho Noweda	Hydrocortisone acetate	1907011-02	1
EuRho/ Anzag	Hydrocortisone acetate	29(1907011-01)	1
Eurho/ Noweda	Hydrocortisone acetate	1703021-01	1
EuRho/ NOWEDA	Hydrocortisone acetate	1805010-01	2
EuRho/ VDL	Hydrocortisone acetate	1706021-01	1
EuRho/AHD	Hydrocortisone acetate	1706021-01	1
EuRho/Alliance Healt	Hydrocortisone acetate	1907011-01	1
EuRho/Gehe	Hydrocortisone acetate	1805010-01	2
EuRho/Kehr	Hydrocortisone acetate	1907011-02	1
Eurho/Noweda	Hydrocortisone acetate	200402902	1
EuRho/Phoenix	Hydrocortisone acetate	1209003-01	1
EuRho/Phönix	Hydrocortisone acetate	2004029-01	1
EuRho	Hydrocortisone acetate	1107004-03	1
Eurho	Hydrocortisone acetate	1706021-01	1
EuRho	Hydrocortisone acetate	1706021-01	1
EuRho	Hydrocortisone acetate	17086212	1
EuRho	Hydrocortisone acetate	1805010-01	7
EuRho	Hydrocortisone acetate	1907011-01	1
EuRho	Hydrocortisone acetate	1907011-02	2
EuRho	Hydrocortisone acetate	2004029-01	3
Euro OT/Anzag	Hydrocortisone acetate	1706021-01	2
Euro OTC	Hydrocortisone acetate		1
Euro OTC	Hydrocortisone acetate	1107004-03	2
Euro OTC	Hydrocortisone acetate	1112031-01	11
Euro OTC	Hydrocortisone acetate	1112031-02	3
Euro OTC	Hydrocortisone acetate	120503401	3
Euro OTC	Hydrocortisone acetate	1205034-01	26
Euro OTC	Hydrocortisone acetate	12090003-01	3
Euro OTC	Hydrocortisone acetate	120900301	2
Euro OTC	Hydrocortisone acetate	1209003-01	20
Euro OTC	Hydrocortisone acetate	1404017-01	13
Euro OTC	Hydrocortisone acetate	1404017-02	6
Euro OTC	Hydrocortisone acetate	1404017-03	1
Euro OTC	Hydrocortisone acetate	140900501	1
Euro OTC	Hydrocortisone acetate	1409005-01	17
Euro OTC	Hydrocortisone acetate	140900502	1
Euro OTC	Hydrocortisone acetate	1409005-02	4
Euro OTC	Hydrocortisone acetate	14301406	1
Euro OTC	Hydrocortisone acetate	1500829-01	1
Euro OTC	Hydrocortisone acetate	150103501	3
Euro OTC	Hydrocortisone acetate	1501035-01	14
Euro OTC	Hydrocortisone acetate	1502000801	1
Euro OTC	Hydrocortisone acetate	1505008	1
Euro OTC	Hydrocortisone acetate	150500801	3
Euro OTC	Hydrocortisone acetate	1505008-01	54

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Hydrocortisone acetate	1508023-01	1
Euro OTC	Hydrocortisone acetate	1508029	2
Euro OTC	Hydrocortisone acetate	150802901	1
Euro OTC	Hydrocortisone acetate	1508029-01	36
Euro OTC	Hydrocortisone acetate	1508029-02	4
Euro OTC	Hydrocortisone acetate	1508029-03	1
Euro OTC	Hydrocortisone acetate	15356903	1
Euro OTC	Hydrocortisone acetate	16004406	2
Euro OTC	Hydrocortisone acetate	160405201	5
Euro OTC	Hydrocortisone acetate	1604052-01	77
Euro OTC	Hydrocortisone acetate	16238707	1
Euro OTC	Hydrocortisone acetate	170602-01	1
Euro OTC	Hydrocortisone acetate	1706021	1
Euro OTC	Hydrocortisone acetate	1706021-0	1
Euro OTC	Hydrocortisone acetate	170602101	1
Euro OTC	Hydrocortisone acetate	1706021-01	84
Euro OTC	Hydrocortisone acetate	17066021-01	1
Euro OTC	Hydrocortisone acetate	170830HA/1706021-01	1
Euro OTC	Hydrocortisone acetate	17086202	1
Euro OTC	Hydrocortisone acetate	17086203	1
Euro OTC	Hydrocortisone acetate	17086204	1
Euro OTC	Hydrocortisone acetate	17219705	1
Euro OTC	Hydrocortisone acetate	17219709	1
Euro OTC	Hydrocortisone acetate	180501001	8
Euro OTC	Hydrocortisone acetate	1805010-01	123
Euro OTC	Hydrocortisone acetate	18050101	1
Euro OTC	Hydrocortisone acetate	1805010-1	1
Euro OTC	Hydrocortisone acetate	18050101-01	1
Euro OTC	Hydrocortisone acetate	180510-01	2
Euro OTC	Hydrocortisone acetate	18142805	1
Euro OTC	Hydrocortisone acetate	18142808	1
Euro OTC	Hydrocortisone acetate	18142811	3
Euro OTC	Hydrocortisone acetate	18278014	1
Euro OTC	Hydrocortisone acetate	1907001-01	1
Euro OTC	Hydrocortisone acetate	1907011	1
Euro OTC	Hydrocortisone acetate	190701101	2
Euro OTC	Hydrocortisone acetate	1907011-01	30
Euro OTC	Hydrocortisone acetate	190701102	2
Euro OTC	Hydrocortisone acetate	1907011-02	27
Euro OTC	Hydrocortisone acetate	1907011-03	8
Euro OTC	Hydrocortisone acetate	19070111-03	1
Euro OTC	Hydrocortisone acetate	1907011-42	1
Euro OTC	Hydrocortisone acetate	1907077-02	1
Euro OTC	Hydrocortisone acetate	19138307	1
Euro OTC	Hydrocortisone acetate	2004029	4
Euro OTC	Hydrocortisone acetate	200402901	1
Euro OTC	Hydrocortisone acetate	2004029-01	52
Euro OTC	Hydrocortisone acetate	2004029-02	10
Euro OTC	Hydrocortisone acetate	2205004_01	1
Euro OTC	Hydrocortisone acetate	2205004-01	18
Euro OTC	Hydrocortisone acetate	2604052-01	1
Euro OTC	Hydrocortisone acetate	30(1805010-01)	1
Euro OTC	Hydrocortisone acetate	31(1907011-01)	1
Euro OTC	Hydrocortisone acetate	508029-01	2
Euro OTC	Hydrocortisone acetate	911I-01718	1
Euro OTC	Hydrocortisone acetate	EuroOTC	2
Euro OTC	Hydrocortisone acetate	HCAZ11004K	1
Euro OTC	Hydrocortisone acetate	K061828180402	1
Euro OTC	Hydrocortisone acetate	L68934	1
Euro/ Sanacorp	Hydrocortisone acetate	1409005-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro/Alliance Healthcare	Hydrocortisone acetate	1508029-01	1
Euro/Gehe	Hydrocortisone acetate	1404017-01	1
Euro/L10	Hydrocortisone acetate	190701101	1
Euro/L10	Hydrocortisone acetate	1907011-01	1
Euro/Noweda	Hydrocortisone acetate	1805010-01	2
Euro/Phönix	Hydrocortisone acetate	1805010	1
Euro/sanacorp	Hydrocortisone acetate	1604052-01	1
Euro/Sanacorp	Hydrocortisone acetate	1805010-01	1
Euroo/Noweda	Hydrocortisone acetate	2004029-01	1
Europh-Gehe	Hydrocortisone acetate	1508029-01	1
EuRro/Anzag	Hydrocortisone acetate	1706021-01	2
Fagro/Gehe	Hydrocortisone acetate	15A07-B03_306545	1
Fagro/Noweda	Hydrocortisone acetate	18142804	1
Fagron	Hydrocortisone acetate		1
Fagron	Hydrocortisone acetate	11/01-N05	1
Fagron	Hydrocortisone acetate	1112031	1
Fagron	Hydrocortisone acetate	12330107	1
Fagron	Hydrocortisone acetate	12K15-N04	6
Fagron	Hydrocortisone acetate	13/31-B07-290061	1
Fagron	Hydrocortisone acetate	13155311	1
Fagron	Hydrocortisone acetate	13A03-N04	4
Fagron	Hydrocortisone acetate	13B25-N04	2
Fagron	Hydrocortisone acetate	13E31-N02	3
Fagron	Hydrocortisone acetate	13E31-No2	1
Fagron	Hydrocortisone acetate	13F25-B05-300290	2
Fagron	Hydrocortisone acetate	13G09-N08	4
Fagron	Hydrocortisone acetate	13J31-B07	3
Fagron	Hydrocortisone acetate	13J31B07290061	1
Fagron	Hydrocortisone acetate	13J31-B07-290061	2
Fagron	Hydrocortisone acetate	13J31-B07-290062	2
Fagron	Hydrocortisone acetate	14043903	1
Fagron	Hydrocortisone acetate	14043905	1
Fagron	Hydrocortisone acetate	14043906	1
Fagron	Hydrocortisone acetate	14144804	1
Fagron	Hydrocortisone acetate	14301402	1
Fagron	Hydrocortisone acetate	14301408	1
Fagron	Hydrocortisone acetate	14A13-B04	1
Fagron	Hydrocortisone acetate	14A13-B04-294158	2
Fagron	Hydrocortisone acetate	14I16-B01-300292	2
Fagron	Hydrocortisone acetate	15067006	1
Fagron	Hydrocortisone acetate	157000-0002	1
Fagron	Hydrocortisone acetate	15A03-B09-307133	1
Fagron	Hydrocortisone acetate	15A03-B09-307300	1
Fagron	Hydrocortisone acetate	15A07-B03-306545	1
Fagron	Hydrocortisone acetate	15A30-B09	1
Fagron	Hydrocortisone acetate	15A30-B09-307133	4
Fagron	Hydrocortisone acetate	15H24-B01	1
Fagron	Hydrocortisone acetate	15h24-b01-314236	1
Fagron	Hydrocortisone acetate	15H24-B01-314236	1
Fagron	Hydrocortisone acetate	15H24-B01-316480	1
Fagron	Hydrocortisone acetate	15I28-B12-316481	1
Fagron	Hydrocortisone acetate	15J28-B12	1
Fagron	Hydrocortisone acetate	15J28-B12-316481	1
Fagron	Hydrocortisone acetate	15J28-b12-317771	1
Fagron	Hydrocortisone acetate	15J28-B12-317771	1
Fagron	Hydrocortisone acetate	16004402	1
Fagron	Hydrocortisone acetate	160405201	1
Fagron	Hydrocortisone acetate	1604052-01	1
Fagron	Hydrocortisone acetate	16238707	1
Fagron	Hydrocortisone acetate	16B03-B04	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Hydrocortisone acetate	16B03-B04-319407	1
Fagron	Hydrocortisone acetate	16B03-B04-320156	1
Fagron	Hydrocortisone acetate	16C15-B04-321458	3
Fagron	Hydrocortisone acetate	16C15-B04-321459	1
Fagron	Hydrocortisone acetate	16H18-B04	2
Fagron	Hydrocortisone acetate	16H18-B04-325093	3
Fagron	Hydrocortisone acetate	16H18B04327324	1
Fagron	Hydrocortisone acetate	16H18-B04-327324	1
Fagron	Hydrocortisone acetate	16h18-b04-327325	1
Fagron	Hydrocortisone acetate	16H18-B04-327325	2
Fagron	Hydrocortisone acetate	16J28-B05	1
Fagron	Hydrocortisone acetate	16J28-B05-330083	1
Fagron	Hydrocortisone acetate	16J28-B51-333889	3
Fagron	Hydrocortisone acetate	17086211	3
Fagron	Hydrocortisone acetate	17219706	1
Fagron	Hydrocortisone acetate	17C10	2
Fagron	Hydrocortisone acetate	17C10-B01-333961	1
Fagron	Hydrocortisone acetate	17C10-B01-333962	5
Fagron	Hydrocortisone acetate	17C10-B01-335774	2
Fagron	Hydrocortisone acetate	17G03	1
Fagron	Hydrocortisone acetate	17G03-B06-338750	1
Fagron	Hydrocortisone acetate	17G03-B06-341304	2
Fagron	Hydrocortisone acetate	17g03-b06-341305	1
Fagron	Hydrocortisone acetate	17G03-B06-341305	2
Fagron	Hydrocortisone acetate	17G03-B06-341843	4
Fagron	Hydrocortisone acetate	17G03-B06-345375	3
Fagron	Hydrocortisone acetate	17G03-B06-345375	1
Fagron	Hydrocortisone acetate	17L19	2
Fagron	Hydrocortisone acetate	17L19-B04	2
Fagron	Hydrocortisone acetate	17L19B04345374	1
Fagron	Hydrocortisone acetate	17L19-B04-345374	1
Fagron	Hydrocortisone acetate	17L19-B04-348983	2
Fagron	Hydrocortisone acetate	17L19-B04-350448	2
Fagron	Hydrocortisone acetate	18142806	1
Fagron	Hydrocortisone acetate	18278005	1
Fagron	Hydrocortisone acetate	18H07	1
Fagron	Hydrocortisone acetate	18H07-B03	3
Fagron	Hydrocortisone acetate	18H07-B03-352228	8
Fagron	Hydrocortisone acetate	18H07-B03-355044	2
Fagron	Hydrocortisone acetate	18H07-B03-356259	4
Fagron	Hydrocortisone acetate	18H07-B03-357240	7
Fagron	Hydrocortisone acetate	18H07-BO3-357240	1
Fagron	Hydrocortisone acetate	19090001	1
Fagron	Hydrocortisone acetate	19A24B05	1
Fagron	Hydrocortisone acetate	19A24-B05	3
Fagron	Hydrocortisone acetate	19A24-B05-359123	1
Fagron	Hydrocortisone acetate	19A24-B05359124	1
Fagron	Hydrocortisone acetate	19A24-B05-359124	7
Fagron	Hydrocortisone acetate	19A24-B05-361623	4
Fagron	Hydrocortisone acetate	19A24-B05-361624	2
Fagron	Hydrocortisone acetate	19A24-BO5-361623	1
Fagron	Hydrocortisone acetate	19J00	1
Fagron	Hydrocortisone acetate	19J10-f04	1
Fagron	Hydrocortisone acetate	19J10-F04	2
Fagron	Hydrocortisone acetate	19J10-F04-36627	1
Fagron	Hydrocortisone acetate	19J10-F04366275	1
Fagron	Hydrocortisone acetate	19J10-F04-366275	2
Fagron	Hydrocortisone acetate	19J10-F04-366276	1
Fagron	Hydrocortisone acetate	19j10-f04-366277	1
Fagron	Hydrocortisone acetate	19J10-F04-366277	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Hydrocortisone acetate	19j10-f04-366278	3
Fagron	Hydrocortisone acetate	19M0-F04-366277	1
Fagron	Hydrocortisone acetate	200508-1	1
Fagron	Hydrocortisone acetate	20804-F07-370096	1
Fagron	Hydrocortisone acetate	20B04-F07	1
Fagron	Hydrocortisone acetate	20B04-F07-370094	2
Fagron	Hydrocortisone acetate	20B04-F07-370095	1
Fagron	Hydrocortisone acetate	20B04-F07-370096	1
Fagron	Hydrocortisone acetate	20F19-F01-371737	1
Fagron	Hydrocortisone acetate	20F19F01371738	1
Fagron	Hydrocortisone acetate	20F19-F01-371740	3
Fagron	Hydrocortisone acetate	20J13-F10	2
Fagron	Hydrocortisone acetate	20J13-F10-375214	2
Fagron	Hydrocortisone acetate	20J13-F10-375216	1
Fagron	Hydrocortisone acetate	20J13-F10-375217	1
Fagron	Hydrocortisone acetate	21d22-f01-378700	1
Fagron	Hydrocortisone acetate	22A17-B07-216283	2
Fagron	Hydrocortisone acetate	22A17-B07-216284	1
Fagron	Hydrocortisone acetate	22A17-B07-216285	3
Fagron	Hydrocortisone acetate	22H11-B01-220314	2
Fagron	Hydrocortisone acetate	2OF19-F01-371737	1
Fagron	Hydrocortisone acetate	32(20F19-F01-371738)	1
Fagron	Hydrocortisone acetate	33(20F19-F01-371738)	1
Fagron	Hydrocortisone acetate	345873/P-19091821	1
Fagron	Hydrocortisone acetate	3613A-01718	1
Fagron	Hydrocortisone acetate	7C10-B01-333961	1
Fagron	Hydrocortisone acetate	8563642	1
Fagron	Hydrocortisone acetate	B05-3591203	1
Fagron	Hydrocortisone acetate	F01-3717308	2
Fagron	Hydrocortisone acetate	F04-3662707	1
Fagron	Hydrocortisone acetate	HC0024	1
Fagron	Hydrocortisone acetate	M39171	1
Fagron	Hydrocortisone acetate	NCEHAC130201	1
Fagron	Hydrocortisone acetate	NCEHAC151101	1
Fagron	Hydrocortisone acetate	NCEHAC170201	2
Fagron	Hydrocortisone acetate	NCEHAC170507	4
Fagron	Hydrocortisone acetate	NCEHAC181105	2
Fagron	Hydrocortisone acetate	NCEHAC1900901	1
Fargon	Hydrocortisone acetate	17L19-B04-345373	1
Fargon	Hydrocortisone acetate	18H07-B03-356259	1
Fargon	Hydrocortisone acetate	19A24-B05-361622	1
Fargon	Hydrocortisone acetate	F01-3717308	1
Fargon	Hydrocortisone acetate	F04-3662705	2
Faron/Noweda	Hydrocortisone acetate	19A24_B05_361622	1
Fiebig	Hydrocortisone acetate	1209003-01	1
Fiebig	Hydrocortisone acetate	1605410	1
Fiebig	Hydrocortisone acetate	16095404	2
Fiebig	Hydrocortisone acetate	17219702	2
Fiebig	Hydrocortisone acetate	17219703	1
Fiebig	Hydrocortisone acetate	18142803	1
Fiebig	Hydrocortisone acetate	18278006	1
Fiebig	Hydrocortisone acetate	18278010	1
Finteler Apotheke	Hydrocortisone acetate	1604052-01	2
Gatt-Koller	Hydrocortisone acetate	1734/05154415	1
Gatt-Koller	Hydrocortisone acetate	1802876	1
GEHE 03.07.2014	Hydrocortisone acetate	14043903	1
Gehe amax	Hydrocortisone acetate	16238712	1
Gehe amax	Hydrocortisone acetate	18142807	2
Gehe amax	Hydrocortisone acetate	18278008	2
Gehe amax	Hydrocortisone acetate	18278019	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe Rostock	Hydrocortisone acetate	20000978010	1
Gehe	Hydrocortisone acetate	1205034-01	1
Gehe	Hydrocortisone acetate	14043905	1
Gehe	Hydrocortisone acetate	14144805	1
Gehe	Hydrocortisone acetate	1501035-01	1
Gehe	Hydrocortisone acetate	15356901	2
Gehe	Hydrocortisone acetate	15356902	1
Gehe	Hydrocortisone acetate	16004408	2
GEHE	Hydrocortisone acetate	1604052-01	1
Gehe	Hydrocortisone acetate	16095407	1
Gehe	Hydrocortisone acetate	16238710	1
GEHE	Hydrocortisone acetate	16238712	1
GEHE	Hydrocortisone acetate	16238713	1
GEHE	Hydrocortisone acetate	1706021-01	2
GEHE	Hydrocortisone acetate	17219703	1
Gehe	Hydrocortisone acetate	17219704	1
Gehe	Hydrocortisone acetate	17219705	3
gehe	Hydrocortisone acetate	17219707	1
Gehe	Hydrocortisone acetate	17219707	3
Gehe	Hydrocortisone acetate	1805010-01	4
Gehe	Hydrocortisone acetate	18142804	1
Gehe	Hydrocortisone acetate	18142812	2
Gehe	Hydrocortisone acetate	18278004	2
Gehe	Hydrocortisone acetate	18278010	1
gehe	Hydrocortisone acetate	18278014	1
GEHE	Hydrocortisone acetate	18278020	1
Gehe	Hydrocortisone acetate	19138305	2
Gehe	Hydrocortisone acetate	19138307	4
Gehe	Hydrocortisone acetate	200004117001	1
Gehe	Hydrocortisone acetate	20000978006	1
Gehe	Hydrocortisone acetate	20000978009	1
Gehe	Hydrocortisone acetate	21002415001	1
Gehe	Hydrocortisone acetate	22002539008	2
Gehe	Hydrocortisone acetate	22002539015	1
GEHE	Hydrocortisone acetate	2205004-01	1
Gehe	Hydrocortisone acetate	2306007-01	1
Geilenkirchen	Hydrocortisone acetate	16238710	1
Geilenkirchen	Hydrocortisone acetate	18142815	1
Geilenkirchen	Hydrocortisone acetate	18278016	1
Geilenkirchen	Hydrocortisone acetate	19138307	1
Geilenkirchen	Hydrocortisone acetate	20000978004	1
Geilenkirchen	Hydrocortisone acetate	20004117004	1
Hedinger/Gehe	Hydrocortisone acetate	1112031-02	1
Hedinger/Sanacorp	Hydrocortisone acetate	1706021-01	2
Henan Lihua Pharma. ...	Hydrocortisone acetate	18142806	1
Henan Lihua Pharmace...	Hydrocortisone acetate	20000978008	1
Henan Lihua Pharmace...	Hydrocortisone acetate	2004029-01	1
Henan/Noweda	Hydrocortisone acetate	K06M20190611	1
Henan/Noweda	Hydrocortisone acetate	KD6M20190612	1
Henan/Phoenix	Hydrocortisone acetate	KO6M20190612	2
Henen / Gehe	Hydrocortisone acetate	20000978004	1
Hepart	Hydrocortisone acetate	14144804	1
Ichthyol GmbH/Noweda	Hydrocortisone acetate	17086205	1
Jenne	Hydrocortisone acetate	21002415006	1
Jenne	Hydrocortisone acetate	23001089005	1
Kehr	Hydrocortisone acetate	1706021-01	2
Kehr	Hydrocortisone acetate	17L19-B04-347866	1
Kehr	Hydrocortisone acetate	22002539008	1
Kehr	Hydrocortisone acetate	22002539010	1
Kehr	Hydrocortisone acetate	22002539013	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Kehr	Hydrocortisone acetate	22002539015	1
Kehr	Hydrocortisone acetate	22H11-B01-224312	1
Kehr	Hydrocortisone acetate	23001089005	2
Klenk	Hydrocortisone acetate	1/06021-01	1
Klenk	Hydrocortisone acetate	1112031-01	1
Klenk	Hydrocortisone acetate	14301401	1
Klenk	Hydrocortisone acetate	18142803	1
Krieger	Hydrocortisone acetate	2205004-01	1
L10	Hydrocortisone acetate	1706021-01	5
L12	Hydrocortisone acetate	1604052-01	3
Lihua/phönix	Hydrocortisone acetate	KO6A20140801M	1
Midas	Hydrocortisone acetate	17219707	1
Nachprüfung	Hydrocortisone acetate		1
Nachprüfung	Hydrocortisone acetate	2082019-4	1
Noveda	Hydrocortisone acetate	20000978008	1
Noweda /Cealo	Hydrocortisone acetate	20000978004	1
Noweda 17.07.2015	Hydrocortisone acetate	14301403	1
Noweda am 10.10.2017	Hydrocortisone acetate	1706021	1
Noweda/ Pharmacia & ...	Hydrocortisone acetate	1205034-01	1
Noweda/apotec	Hydrocortisone acetate	2205004-01	1
Noweda/Euro	Hydrocortisone acetate	1501035-01	1
Noweda	Hydrocortisone acetate	1112031-02	1
Noweda	Hydrocortisone acetate	13G09-N08	1
Noweda	Hydrocortisone acetate	16095407	1
Noweda	Hydrocortisone acetate	16095410	2
Noweda	Hydrocortisone acetate	16238710	1
Noweda	Hydrocortisone acetate	17219705	1
Noweda	Hydrocortisone acetate	17219706	1
Noweda	Hydrocortisone acetate	17219707	4
Noweda	Hydrocortisone acetate	18142804	2
Noweda	Hydrocortisone acetate	18142805	2
Noweda	Hydrocortisone acetate	18142806	1
Noweda	Hydrocortisone acetate	18142807	1
Noweda	Hydrocortisone acetate	18142808	1
Noweda	Hydrocortisone acetate	18278004	2
Noweda	Hydrocortisone acetate	18278010	1
Noweda	Hydrocortisone acetate	18278014	2
Noweda	Hydrocortisone acetate	18278015	1
Noweda	Hydrocortisone acetate	18278019	3
Noweda	Hydrocortisone acetate	1907011-01	1
Noweda	Hydrocortisone acetate	19138303	1
Noweda	Hydrocortisone acetate	20000978005	1
Noweda	Hydrocortisone acetate	20000978010	1
Noweda	Hydrocortisone acetate	20004117005	2
Noweda	Hydrocortisone acetate	20004117007	1
Noweda	Hydrocortisone acetate	20004278004	1
Noweda	Hydrocortisone acetate	21002415011	1
Noweda	Hydrocortisone acetate	21002415014	1
Noweda	Hydrocortisone acetate	2200253900	1
Noweda	Hydrocortisone acetate	22002539001	1
Noweda	Hydrocortisone acetate	22002539004	1
Noweda	Hydrocortisone acetate	22002539005	3
Noweda	Hydrocortisone acetate	22002539008	2
Noweda	Hydrocortisone acetate	22002539012	2
Noweda	Hydrocortisone acetate	22002539013	1
Noweda	Hydrocortisone acetate	22002539014	1
Noweda	Hydrocortisone acetate	22002539015	1
noweda	Hydrocortisone acetate	2205004	1
Noweda	Hydrocortisone acetate	2205004-01	1
Noweda	Hydrocortisone acetate	23001089004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Hydrocortisone acetate	caelo	1
Otto Fischer GmbH&Co...	Hydrocortisone acetate	1907011-02	3
ph euro	Hydrocortisone acetate	1907011-01	1
ph euro	Hydrocortisone acetate	1907011-02	1
Pharmacia&Upjohn Com...	Hydrocortisone acetate	1209003-01	1
Phoenix 14.01.2015 E...	Hydrocortisone acetate	14043902	1
Phoenix 24.01.2019	Hydrocortisone acetate	18278004	1
Phoenix Goettin	Hydrocortisone acetate	1209003-01	1
Phoenix	Hydrocortisone acetate	1209003-01	1
Phoenix	Hydrocortisone acetate	12182402	1
Phoenix	Hydrocortisone acetate	12330107	1
Phoenix	Hydrocortisone acetate	1568/05131813	1
Phoenix	Hydrocortisone acetate	15A30-B09	1
Phoenix	Hydrocortisone acetate	15J28-B12	1
Phoenix	Hydrocortisone acetate	16004403	1
Phoenix	Hydrocortisone acetate	17086204	2
Phoenix	Hydrocortisone acetate	17086205	1
Phoenix	Hydrocortisone acetate	18142802	1
Phoenix	Hydrocortisone acetate	18278015	1
Phoenix	Hydrocortisone acetate	18278016	2
Phoenix	Hydrocortisone acetate	18H07-B03-352227	1
Phoenix	Hydrocortisone acetate	1907011-03	2
Phoenix	Hydrocortisone acetate	19138304	1
Phoenix	Hydrocortisone acetate	20000978004	1
Phoenix	Hydrocortisone acetate	20004117001	1
Phoenix	Hydrocortisone acetate	20004278004	1
Phoenix	Hydrocortisone acetate	20004278008	1
Phoenix	Hydrocortisone acetate	200303103	1
Phoenix	Hydrocortisone acetate	2004029-01	2
Phoenix	Hydrocortisone acetate	200421105	1
Phoenix	Hydrocortisone acetate	22002539019	1
Phoenix	Hydrocortisone acetate	23001089004	2
Phoenix	Hydrocortisone acetate	3068	1
Phoenix	Hydrocortisone acetate	3209	1
Phönix Gotha	Hydrocortisone acetate	12182405	1
Phönix Gotha	Hydrocortisone acetate	12330108	1
Phönix Gotha	Hydrocortisone acetate	17219706	1
Phönix, Caesar&Loret...	Hydrocortisone acetate	191383001	1
Phönix/Lihua	Hydrocortisone acetate	1409005-01	1
Phönix	Hydrocortisone acetate	1112031-01	1
Phönix	Hydrocortisone acetate	1112031-02	1
Phönix	Hydrocortisone acetate	1205034-01	1
Phönix	Hydrocortisone acetate	12182405	1
Phönix	Hydrocortisone acetate	12A13-N02	1
Phönix	Hydrocortisone acetate	12K15-No4	1
Phönix	Hydrocortisone acetate	14144804	2
phönix	Hydrocortisone acetate	15356901	2
phönix	Hydrocortisone acetate	16238708	1
phönix	Hydrocortisone acetate	16238712	1
Phönix	Hydrocortisone acetate	1706021-01	1
PHÖNIX	Hydrocortisone acetate	17086211	1
Phönix	Hydrocortisone acetate	17219705	1
Phönix	Hydrocortisone acetate	1805010-01	1
Phönix	Hydrocortisone acetate	18142802	1
phönix	Hydrocortisone acetate	18142804	1
Phönix	Hydrocortisone acetate	18142815	2
Phönix	Hydrocortisone acetate	18278004	2
Phönix	Hydrocortisone acetate	18278005	1
Phönix	Hydrocortisone acetate	18278006	1
Phönix	Hydrocortisone acetate	18278010	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Hydrocortisone acetate	18278014	1
Phönix	Hydrocortisone acetate	18278016	1
Phönix	Hydrocortisone acetate	19138302	3
PHÖNIX	Hydrocortisone acetate	19138305	1
Phönix	Hydrocortisone acetate	19138307	1
Phönix	Hydrocortisone acetate	20000978004	1
Phönix	Hydrocortisone acetate	20000978006	1
Phönix	Hydrocortisone acetate	20000978010	1
phonix	Hydrocortisone acetate	20004117001	1
Phönix	Hydrocortisone acetate	20004278002	1
Phönix	Hydrocortisone acetate	20004278003	1
PHÖNIX	Hydrocortisone acetate	20004278003	1
Phönix	Hydrocortisone acetate	20004278004	1
Phönix	Hydrocortisone acetate	2000978007	1
Phönix	Hydrocortisone acetate	2000978009	1
Phönix	Hydrocortisone acetate	2004029-01	4
PHÖNIX	Hydrocortisone acetate	21002415001	2
Phönix	Hydrocortisone acetate	21002415002	1
Phönix	Hydrocortisone acetate	21002415004	2
Phönix	Hydrocortisone acetate	22002539014	1
Phönix	Hydrocortisone acetate	22002539019	4
Phönix	Hydrocortisone acetate	AKD8	1
Röntgen	Hydrocortisone acetate	16095410	1
Röntgen	Hydrocortisone acetate	17219705	1
Röntgen	Hydrocortisone acetate	18278010	1
Röntgen	Hydrocortisone acetate	19138307	1
Röntgen	Hydrocortisone acetate	20000977002	1
Röntgen	Hydrocortisone acetate	21002415010	1
Sanacorp	Hydrocortisone acetate	1107004-03	1
Sanacorp	Hydrocortisone acetate	11263913	1
Sanacorp	Hydrocortisone acetate	12182404	2
Sanacorp	Hydrocortisone acetate	12330103	1
Sanacorp	Hydrocortisone acetate	13155302	2
Sanacorp	Hydrocortisone acetate	13291704	1
Sanacorp	Hydrocortisone acetate	14043903	1
Sanacorp	Hydrocortisone acetate	1409005-01	3
sanacorp	Hydrocortisone acetate	14301406	1
Sanacorp	Hydrocortisone acetate	1501035-01	1
Sanacorp	Hydrocortisone acetate	16095407	1
Sanacorp	Hydrocortisone acetate	16238706	1
Sanacorp	Hydrocortisone acetate	16238708	1
Sanacorp	Hydrocortisone acetate	16238710	1
Sanacorp	Hydrocortisone acetate	1706021-01	1
Sanacorp	Hydrocortisone acetate	17219704	1
Sanacorp	Hydrocortisone acetate	17219708	1
Sanacorp	Hydrocortisone acetate	18142805	2
Sanacorp	Hydrocortisone acetate	18278006	1
Sanacorp	Hydrocortisone acetate	18278008	3
Sanacorp	Hydrocortisone acetate	185010-01	1
Sanacorp	Hydrocortisone acetate	191383004	1
Sanacorp	Hydrocortisone acetate	20004117006	1
Sanacorp	Hydrocortisone acetate	20004278003	6
Sanacorp	Hydrocortisone acetate	20004278009	1
Sanacorp	Hydrocortisone acetate	21002415001	1
Sanacorp	Hydrocortisone acetate	22002539002	1
Sanacorp	Hydrocortisone acetate	22002539008	1
Sanacorp	Hydrocortisone acetate	22002539009	2
Sanacorp	Hydrocortisone acetate	22002539010	1
Sanacorp	Hydrocortisone acetate	23001089006	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Hydrocortisone acetate	2306007-01	3
SanacorpWE:13.02.201…	Hydrocortisone acetate	1604052-01	1
sannacop	Hydrocortisone acetate	2205004-01	1
Tianjin Jinjin Pharm…	Hydrocortisone acetate	19138304	1
Tianjin Jinjin Pharm…	Hydrocortisone acetate	18278019	1
Tianjin Jinjin/Gehe	Hydrocortisone acetate	17L19-B04-345373	1
Tianjin/Noweda	Hydrocortisone acetate	HD0027	1
Tianjin/Noweda	Hydrocortisone acetate	HD0039	2
Wepa/Noweda	Hydrocortisone acetate	20004117001	1
xxx	Hydrocortisone acetate		1

- 230 479 spectra from 1515 *Apo-Ident* customers from a total of 48 671 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hydrocortisone acetate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hydrocortisone acetate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	429	0	152 533
Type B	0	1296	0	200 788
Type C	0	5548	40	230 479

The substance/substance group *Hydrocortisone acetate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6014 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.5370 %)
Type C	100.0000 % (> 99.9007 %)	99.2842 % (> 99.2305 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21295	21889	6.84	178.22
21462	21889	6.07	178.07
21889	21889	0.00	180.82
22241	21889	4.70	179.00
22564	22564	0.00	182.94
24392	24392	0.00	179.29
24590	22564	8.23	182.48

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hydroquinone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20091-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hydroquinone; Hydrochinonum

Special notes

When selecting the *Hydroquinone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hydroquinone	8	4	82

Second-stage model

For differentiation of the substance/substance group *Hydroquinone* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hydroquinone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Resocrinol	44.48	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hydroquinone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hydroquinone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hydroquinone	12288505	20884	40	20121015
Caelo	Hydroquinone	14026904	21468	60	20140122
Caelo	Hydroquinone	14281501	21791	60	AR-15-FG-008058-01
Caelo	Hydroquinone	14280110	21923	60	20141017
Caelo	Hydroquinone	15057001	22324	60	20150306
Caelo	Hydroquinone	15057001	22351	60	20150306
Caelo	Hydroquinone	182306	24761	40	20181008*
Caelo	Hydroquinone	192642	24890	40	20191115*
Gatt-Koller	Hydroquinone	23J02483	27097	30	20240109
Gatt-Koller	Hydroquinone	23J02483	27097SI	20	20240109

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 470 spectra of 10 reference samples from the substance/substance group *Hydroquinone*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 492 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 5 reference samples from the substance/substance group *Hydroquinone*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydroquinone	15057004	21975	60
Caelo	Hydroquinone	16023105	23114	40
Caelo	Hydroquinone	172215	23654	40
Caelo	Hydroquinone	23000425	27226	40
Caelo	Hydroquinone	23000425	27226SI	20

- 201 884 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 524 spectra from 337 *Apo-Ident* customers from 90 batches from the substance/substance group *Hydroquinone*.

- Among them are spectra of independent samples from 82 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Hydroquinone	20001617007	2
	Hydroquinone	21003639007	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
	Hydroquinone	21003639008	1
	Hydroquinone	21003639010	3
	Hydroquinone	21003639011	5
14026902	Hydroquinone	InterneCharge1214Q	1
16023112	Hydroquinone	16023112	1
A.H. 14.06.13 ek: 3,97EUR	Hydroquinone	12288505	1
ACM	Hydroquinone	KNC0635J17	1
ACM	Hydroquinone	KNC1047J15	2
AHD	Hydroquinone	13105405	1
AHD	Hydroquinone	21003639010	1
AHL	Hydroquinone	16023102	1
Alli	Hydroquinone	21003639010	1
Alliance Healthcare	Hydroquinone	20001617007	1
Allianz	Hydroquinone	16023116	1
Anzag	Hydroquinone	12156705	1
Anzag	Hydroquinone	12288505	2
apomix	Hydroquinone	13105408	1
Caelo	Hydroquinone		3
Caelo	Hydroquinone	1(192642008)0	1
Caelo	Hydroquinone	10145101	1
Caelo	Hydroquinone	10145103	1
Caelo	Hydroquinone	10145113	2
Caelo	Hydroquinone	11163905	5
Caelo	Hydroquinone	11163907	5
Caelo	Hydroquinone	11163912	4
Caelo	Hydroquinone	11163912/Int312052	1
Caelo	Hydroquinone	1163902	1
Caelo	Hydroquinone	12156703	1
Caelo	Hydroquinone	12156705	5
Caelo	Hydroquinone	12156706	1
Caelo	Hydroquinone	1228503	1
Caelo	Hydroquinone	12288502	2
Caelo	Hydroquinone	12288503	2
Caelo	Hydroquinone	12288505	11
Caelo	Hydroquinone	1263912	1
Caelo	Hydroquinone	13105402	5
Caelo	Hydroquinone	13105405	6
Caelo	Hydroquinone	13105408	7
Caelo	Hydroquinone	14026902	5
Caelo	Hydroquinone	14026904	1
Caelo	Hydroquinone	1410401	1
Caelo	Hydroquinone	14121202	1
Caelo	Hydroquinone	14180401	4
Caelo	Hydroquinone	14180406	3
Caelo	Hydroquinone	14180410	4
Caelo	Hydroquinone	14280104	5
Caelo	Hydroquinone	14280105	2
Caelo	Hydroquinone	14281501	11
Caelo	Hydroquinone	14281504	1
Caelo	Hydroquinone	14281507	4
Caelo	Hydroquinone	15023105	1
Caelo	Hydroquinone	15057001	11
Caelo	Hydroquinone	15057002	1
Caelo	Hydroquinone	15057004	13
Caelo	Hydroquinone	15057010	17
Caelo	Hydroquinone	160123118	1
Caelo	Hydroquinone	160223105	1
Caelo	Hydroquinone	16023102	3
Caelo	Hydroquinone	16023105	16
Caelo	Hydroquinone	16023112	11

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hydroquinone	16023113	9
Caelo	Hydroquinone	160231135430	1
Caelo	Hydroquinone	16023116	25
Caelo	Hydroquinone	16023118	16
Caelo	Hydroquinone	16023118P-190314-1	1
Caelo	Hydroquinone	16051502	1
Caelo	Hydroquinone	17221503	1
Caelo	Hydroquinone	17221508	10
Caelo	Hydroquinone	18017902	28
Caelo	Hydroquinone	18017905	9
Caelo	Hydroquinone	1801792	1
Caelo	Hydroquinone	18031403	1
Caelo	Hydroquinone	18230602	15
Caelo	Hydroquinone	18230607	10
Caelo	Hydroquinone	192642003	26
Caelo	Hydroquinone	192642008	4
Caelo	Hydroquinone	20001617002	10
Caelo	Hydroquinone	20001617004	1
Caelo	Hydroquinone	20001617005	6
Caelo	Hydroquinone	20001617007	18
Caelo	Hydroquinone	2000167007	1
Caelo	Hydroquinone	20101806	1
Caelo	Hydroquinone	20200712-3	1
Caelo	Hydroquinone	21003639007	3
Caelo	Hydroquinone	21003639010	1
Caelo	Hydroquinone	21102014A	1
Caelo	Hydroquinone	3281	1
Caelo	Hydroquinone	4017A-01717	1
Caelo	Hydroquinone	52840166	1
Caelo	Hydroquinone	8725	1
Caelo	Hydroquinone	8816-10-583	1
Caeolo/Gehe	Hydroquinone	16023116	1
Caeolo	Hydroquinone	16023105	1
Caesar & Loretz GmbH...	Hydroquinone	18017902	1
Caesar & Loretz GmbH...	Hydroquinone	192642003	1
Caesar & Loretz GmbH...	Hydroquinone	11163912	1
Caesar & Loretz GmbH...	Hydroquinone	18017902	1
Caesar & Loretz GmbH...	Hydroquinone	20001617002	1
Caesar & Loretz GmbH...	Hydroquinone	18230607	1
Caesar & Loretz GmbH...	Hydroquinone	20001617007	1
Caesar & Loretz GmbH...	Hydroquinone	192642003	1
Caesar & Loretz GmbH...	Hydroquinone	20001617002	1
Caesar & Loretz GmbH...	Hydroquinone	20001617002	1
Caesar & Loretz GmbH	Hydroquinone	13105405	1
Caesar & Loretz GmbH	Hydroquinone	16023105	1
Caesar & Loretz GmbH	Hydroquinone	18017902	3
Caesar & Loretz GmbH	Hydroquinone	18230602	4
Caesar & Loretz GmbH	Hydroquinone	18230607	1
Caesar & Loretz GmbH	Hydroquinone	192642003	8
Caesar & Loretz GmbH	Hydroquinone	192642008	2
Caesar & Loretz GmbH	Hydroquinone	20001617002	6
Caesar & Loretz GmbH	Hydroquinone	20001617005	2
Caesar & Loretz GmbH	Hydroquinone	20001617006	1
Caesar & Loretz GmbH	Hydroquinone	20001617007	9
Caesar & Loretz GmbH	Hydroquinone	21003639002	1
Caesar & Loretz GmbH	Hydroquinone	21003639007	2
Caesar & Loretz GmbH	Hydroquinone	21003639010	2
Caesar & Loretz Hilden	Hydroquinone	20001617002	1
Caesar & Loretz	Hydroquinone	16023112	1
Caesar & Loretz	Hydroquinone	192642008	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar / Gehe	Hydroquinone	16023116	1
Caesar und Loretz	Hydroquinone	18230607	1
Cealo	Hydroquinone	192642003	1
Cesar&Loretz GmbH	Hydroquinone	192642008	1
E Plus	Hydroquinone	18017902	1
Euro OTC	Hydroquinone	16023118	2
Euro/Sanacorp	Hydroquinone	15057004	1
Fagron	Hydroquinone		1
Fiebig	Hydroquinone	16023116	1
Gatt-Koller	Hydroquinone	1803302	4
Gatt-Koller	Hydroquinone	22J00202	1
Gehe/Gehe	Hydroquinone	14280110	1
Gehe	Hydroquinone	12156706	2
GEHE	Hydroquinone	16023105	1
GEHE	Hydroquinone	16023118	1
GEHE	Hydroquinone	18017902	1
Gehe	Hydroquinone	21003639007	2
Gehe	Hydroquinone	21003639010	1
Kehr	Hydroquinone	16023112	1
Kehr	Hydroquinone	16023113	1
Noweda	Hydroquinone	16023116	2
noweda	Hydroquinone	18230602	1
Noweda	Hydroquinone	21003639010	1
Phoenix Goettin	Hydroquinone	14281501	1
Phoenix	Hydroquinone	16023105	1
Phoenix	Hydroquinone	18017905	1
Phoenix	Hydroquinone	18230602	1
Phoenix	Hydroquinone	192642003	1
Phoenix	Hydroquinone	200671007	1
Phönix	Hydroquinone	12288503	2
Phönix	Hydroquinone	13105408	1
phönix	Hydroquinone	16023105	1
Sanacorp	Hydroquinone	12156703	1
Sanacorp	Hydroquinone	12288503	1
Sanacorp	Hydroquinone	16023103	1
Sanacorp	Hydroquinone	16023118	1
Sanacorp	Hydroquinone	18230602	1
Sanacorp	Hydroquinone	18230607	1
Sanacorp	Hydroquinone	21003639007	1
Sanacorp	Hydroquinone	23000425005	1
Sanacorp	Hydroquinone	5118M-01717	1

- 235 543 spectra from 1515 *Apo-Ident* customers from a total of 49 170 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hydroquinone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hydroquinone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	470	0	152 492
Type B	0	200	0	201 884
Type C	0	505	19	235 543

The substance/substance group *Hydroquinone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7234 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9007 %)	96.3740 % (> 95.8015 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20884	21791	3.62	64.66
21468	21791	11.38	62.44
21791	21791	0.00	62.27
21923	21791	5.55	62.32
22324	21791	5.03	60.77
22351	21791	3.89	60.76
24761	24761	0.00	62.02
24890	24890	0.00	63.08
27097	21791	15.52	70.20

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hydroxyethyl cellulose**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10006129-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hydroxyethyl cellulose; Hydroxyethylcellulosum

Special notes

When selecting the *Hydroxyethyl cellulose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hydroxyethyl cellulose	9	38	0

Second-stage model

For differentiation of the substance/substance group *Hydroxyethyl cellulose* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hydroxyethyl cellulose* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	88.51	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hydroxyethyl cellulose* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hydroxyethyl cellulose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hydroxyethyl cellulose	181131	26775	40	20180612*
Caelo	Hydroxyethyl cellulose	22002812	26779	40	20221031*
Caelo	Hydroxyethyl cellulose	22002812	26779SI	20	20221031*
Caelo	Hydroxyethyl cellulose	23000202	26781	40	20230210*
Caelo	Hydroxyethyl cellulose	23000202	26781SI	20	20230210*
Caelo	Hydroxyethyl cellulose	13378506	26785	40	1507205
Caelo	Hydroxyethyl cellulose	12274720	26789	20	20121001
Caelo	Hydroxyethyl cellulose	171151	26793	40	20170523*
Caelo	Hydroxyethyl cellulose	22000306	26812	40	20220314*
Euro OTC	Hydroxyethyl cellulose	2306013	26884	40	20230801*
Euro OTC	Hydroxyethyl cellulose	2408008	27390	40	20241008*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 380 spectra of 11 reference samples from the substance/substance group *Hydroxyethyl cellulose*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 582 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1710 spectra of 45 reference samples from the substance/substance group *Hydroxyethyl cellulose*.

- Among them are spectra of independent samples from 38 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydroxyethyl cellulose	190174	26774	40
Caelo	Hydroxyethyl cellulose	191675	26776	40
Caelo	Hydroxyethyl cellulose	20000136	26777	40
Caelo	Hydroxyethyl cellulose	22000131	26778	40
Caelo	Hydroxyethyl cellulose	12249204	26782	40
Caelo	Hydroxyethyl cellulose	14352504	26790	60
Caelo	Hydroxyethyl cellulose	161006	26791	60
Caelo	Hydroxyethyl cellulose	16012909	26792	40
Caelo	Hydroxyethyl cellulose	16252003	26794	40
Caelo	Hydroxyethyl cellulose	16252008	26795	40
Caelo	Hydroxyethyl cellulose	16278705	26796	40
Caelo	Hydroxyethyl cellulose	173196	26798	40
Caelo	Hydroxyethyl cellulose	17115103	26799	40
Caelo	Hydroxyethyl cellulose	190769	26802	40
Caelo	Hydroxyethyl cellulose	190767	26803	40
Caelo	Hydroxyethyl cellulose	192602	26806	40
Caelo	Hydroxyethyl cellulose	21001636	26810	50
Caelo	Hydroxyethyl cellulose	20004006004	26811	40
Caelo	Hydroxyethyl cellulose	23001448	26854	40
Caelo	Hydroxyethyl cellulose	23002026	26966	40
Caelo	Hydroxyethyl cellulose	24001032	27220	40
Euro OTC	Hydroxyethyl cellulose	2211007	26780	40
Euro OTC	Hydroxyethyl cellulose	1110024-04	26783	40
Euro OTC	Hydroxyethyl cellulose	1606030	26786	40
Euro OTC	Hydroxyethyl cellulose	1610039	26787	40
Euro OTC	Hydroxyethyl cellulose	1711012	26800	40
Euro OTC	Hydroxyethyl cellulose	1804003	26801	40
Euro OTC	Hydroxyethyl cellulose	1907013	26804	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Hydroxyethyl cellulose	1911004	26805	40
Euro OTC	Hydroxyethyl cellulose	2008018	26807	40
Euro OTC	Hydroxyethyl cellulose	2101017	26808	40
Euro OTC	Hydroxyethyl cellulose	2302006	26814	40
Euro OTC	Hydroxyethyl cellulose	2305002	26815	40
Fagron	Hydroxyethyl cellulose	13H22-N11	26784	40
Fagron	Hydroxyethyl cellulose	16E09-B05-327042	26788	40
Fagron	Hydroxyethyl cellulose	20H03-B06-197061	26809	50
Fagron	Hydroxyethyl cellulose	21G14-B02-213646	26813	40
Fagron	Hydroxyethyl cellulose	23E11-B01-232178	26986	40
Caelo	Hydroxyethyl cellulose	22000131	26778SI	10
Caelo	Hydroxyethyl cellulose	16278705	26797	40
Caelo	Hydroxyethyl cellulose	20004006004	26811SI	10
Caelo	Hydroxyethyl cellulose	22000306	26812SI[†]	10
Euro OTC	Hydroxyethyl cellulose	2211007	26780SI	20
Euro OTC	Hydroxyethyl cellulose	2302006	26814SI	20
Fagron	Hydroxyethyl cellulose	21G14-B02-213646	26813SI	20

- 200 374 spectra from a total of 4006 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Hydroxyethyl cellulose*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hydroxyethyl cellulose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hydroxyethyl cellulose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	1710	0	200 374
Type C	0	0	0	236 067

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The substance/substance group *Hydroxyethyl cellulose* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.6491 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26775	26775	0.00	136.25
26779	26779	0.00	161.13
26781	26781	0.00	150.86
26785	26785	0.00	170.24
26789	26781	49.90	176.03
26793	26793	0.00	148.13
26812	26812	0.00	190.85
26884	26884	0.00	174.03
27390	27390	0.00	184.27

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hyoscine butylbromide**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20766-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hyoscine butylbromide; Hyoscini butylbromidum

Special notes

When selecting the *Hyoscine butylbromide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hyoscine butylbromide	6	4	2

Second-stage model

For differentiation of the substance/substance group *Hyoscine butylbromide* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hyoscine butylbromide* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	115.97	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hyoscine butylbromide* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hyoscine butylbromide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Hyoscine butylbromide	12K01-N07	20766	40	1406057
Fagron	Hyoscine butylbromide	12K01-N07	20897	40	20121102
Fagron	Hyoscine butylbromide	13K22-N03	21049	40	20131126
Fagron	Hyoscine butylbromide	15I09-B04-312245	21954	60	20150921
Fagron	Hyoscine butylbromide	18A03-B01-352889	24576	40	20180122
Fagron	Hyoscine butylbromide	21K26-B03-221816	26294	40	20220226
Fagron	Hyoscine butylbromide	23G12-B15-233752	26982	40	20230808

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 300 spectra of 7 reference samples from the substance/substance group *Hyoscine butylbromide*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 662 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 270 spectra of 8 reference samples from the substance/substance group *Hyoscine butylbromide*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Hyoscine butylbromide	15I09-B04-316806	22344	60
Fagron	Hyoscine butylbromide	16I20-B08-326942	22903	40
Fagron	Hyoscine butylbromide	20C24-F01-369374	25482	40
Fagron	Hyoscine butylbromide	21B12-F02-377294	25911	40
Fagron	Hyoscine butylbromide	16I20-B08-326942	22937	40
Fagron	Hyoscine butylbromide	21B12-F02-377294	25911SI	10
Fagron	Hyoscine butylbromide	21K26-B03-221816	26294SI†	20
Fagron	Hyoscine butylbromide	23G12-B15-233752	26982SI†	20

- 201 814 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 15 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Hyoscine butylbromide*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
Fagron	Hyoscine butylbromide	16I20-B08-326942	12
Fagron	Hyoscine butylbromide	18A03-B01-352889	2
Fagron	Hyoscine butylbromide	21B12-F02-377294	1

- 236 052 spectra from 1515 *Apo-Ident* customers from a total of 49 255 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hyoscine butylbromide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hyoscine butylbromide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	270	0	201 814
Type C	0	15	0	236 052

The substance/substance group *Hyoscine butylbromide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.7778 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20766	20766	0.00	249.58
20897	20766	43.50	247.83
21049	20766	9.22	247.88
21954	20766	8.99	248.71

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24576	20766	20.20	248.95
26294	20766	18.94	249.50
26982	20766	15.19	250.25

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Hyoscine hydrobromide**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21676-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Hyoscine hydrobromide; Scopolamini hydrobromidum

Special notes

When selecting the *Hyoscine hydrobromide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Hyoscine hydrobromide	7	3	28

Second-stage model

For differentiation of the substance/substance group *Hyoscine hydrobromide* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Hyoscine hydrobromide* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	78.09	–
⋮	⋮	⋮
Riboflavin	>50	57.82
Tosylchloramide sodium	>50	69.01
Polymyxin B sulfate	>50	71.00
Bacitracin	>50	86.91
Colistin sulfate	>50	90.05
Cyanocobalamin	>50	95.64
Amphotericin B	>50	126.25
Calcium pantothenate	>50	139.48
Triamcinolone	>50	145.90
Estriol	>50	151.58
Estradiol hemihydrate	>50	158.98
Nystatin	>50	168.80
alpha-tocopheryl acetate dry concentrate	>50	188.51
Calcium glycerophosphate	>50	207.79
Methylcobalamin	>50	216.14
SyrSpend® SF pH4 neo (Maize starch)	>50	232.83
Oxalic acid	>50	250.88
SyrSpend® SF Alka	>50	267.51
Gelatine, white	>50	277.11
Selenium yeast	>50	284.21
Rice starch	>50	312.06
Carmellose sodium	>50	360.42
Wheat starch	>50	394.99
SyrSpend® SF pH4	>50	470.03
Potato starch	>50	487.35
Fructose	>50	519.47
Corn starch	>50	529.02
Acacia, dried dispersion	>50	536.12
Maltodextrin	>50	637.18

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Hyoscine hydrobromide* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Hyoscine hydrobromide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hyoscine hydrobromide	14278801	21676	60	1504154
Caelo	Hyoscine hydrobromide	15054501	21764	60	1511156
Caelo	Hyoscine hydrobromide	15054501	21764SI	28	1511156
Caelo	Hyoscine hydrobromide	190869	24880	40	20190604*
Caelo	Hyoscine hydrobromide	190869	24880SI	40	20190604*
Caelo	Hyoscine hydrobromide	172303	24881	40	20170926*
Caelo	Hyoscine hydrobromide	21001472001	25733	40	20210423
Caelo	Hyoscine hydrobromide	21001472001	25733SI	40	20210423
Fagron	Hyoscine hydrobromide	15L09-B04-334706	23418	40	20151228
Fagron	Hyoscine hydrobromide	15L09-B04-334706	23418SI	40	20151228
Fagron	Hyoscine hydrobromide	15L09-B04-334706	23419	40	20151228
Fagron	Hyoscine hydrobromide	15L09-B04-334706	23419SI	40	20151228
Fagron	Hyoscine hydrobromide	19G29-B02-367045	25042	40	20191223

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 548 spectra of 13 reference samples from the substance/substance group *Hyoscine hydrobromide*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 414 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 442 spectra of 11 reference samples from the substance/substance group *Hyoscine hydrobromide*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hyoscine hydrobromide	15054504	21925	60
Caelo	Hyoscine hydrobromide	22003532001	26474	40
Fagron	Hyoscine hydrobromide	21G10-B13-221851	26323	40
Caelo	Hyoscine hydrobromide	15054501	21764SI†	32
Caelo	Hyoscine hydrobromide	15054504	21925SI	30
Caelo	Hyoscine hydrobromide	15054504	23441	40
Caelo	Hyoscine hydrobromide	15054504	23441SI	40
Caelo	Hyoscine hydrobromide	172303	24881SI†	40
Caelo	Hyoscine hydrobromide	22003532001	26474SI	40
Fagron	Hyoscine hydrobromide	19G29-B02-367045	25042SI†	40
Fagron	Hyoscine hydrobromide	21G10-B13-221851	26323SI	40

- 201 642 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 75 spectra from 33 *Apo-Ident* customers from 30 batches from the substance/substance group *Hyoscine hydrobromide*.

- Among them are spectra of independent samples from 28 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Hyoscine hydrobromide	22003532001	1
	Hyoscine hydrobromide	22003532004	2
Caelo	Hyoscine hydrobromide	14278801	26
Caelo	Hyoscine hydrobromide	15054505	1
Caelo	Hyoscine hydrobromide	15054511	1
Caelo	Hyoscine hydrobromide	15358901	1
Caelo	Hyoscine hydrobromide	16206204	1
Caelo	Hyoscine hydrobromide	16206208	1
Caelo	Hyoscine hydrobromide	17230303	2
Caelo	Hyoscine hydrobromide	18024806	4
Caelo	Hyoscine hydrobromide	18024807	4
Caelo	Hyoscine hydrobromide	190869002	1
Caelo	Hyoscine hydrobromide	19086901	5
Caelo	Hyoscine hydrobromide	20001949001	4
Caelo	Hyoscine hydrobromide	21000424002	1
Caesar & Loretz GmbH	Hyoscine hydrobromide	20001949001	1
Caesar & Loretz GmbH	Hyoscine hydrobromide	21001472001	1
Caesar & Loretz GmbH	Hyoscine hydrobromide	22000116002	1
Fagron	Hyoscine hydrobromide	14F11-B02-296840	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Hyoscine hydrobromide	14J27-B05-307020	2
Fagron	Hyoscine hydrobromide	15L09-B04-327494	1
Fagron	Hyoscine hydrobromide	17D18-B05-335528	2
Fagron	Hyoscine hydrobromide	18B23-B04-357420	1
Fagron	Hyoscine hydrobromide	19G29-B02	1
Fagron	Hyoscine hydrobromide	21G28-F04	1
Fagron	Hyoscine hydrobromide	21G28-F04-379942	1
Fagron	Hyoscine hydrobromide	21G28-F04-379944	2
Fagron	Hyoscine hydrobromide	2630421	1
Fagron	Hyoscine hydrobromide	B02-3670405	1
Gehe	Hyoscine hydrobromide	19086901	1
Phönix	Hyoscine hydrobromide	19869002	1
Sanacorp	Hyoscine hydrobromide	2100424002	1

- 235 992 spectra from 1515 *Apo-Ident* customers from a total of 49 228 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Hyoscine hydrobromide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Hyoscine hydrobromide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	548	0	152 414
Type B	0	442	0	201 642
Type C	0	75	0	235 992

The substance/substance group *Hyoscine hydrobromide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9051 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6425 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 92.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested

reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21676	21676	0.00	94.08
21764	21764	0.00	87.00
23418	21764	44.31	127.76
23419	21764	45.98	133.52
24880	24880	0.00	94.65
24881	24881	0.00	71.70
25042	21676	7.53	96.36
25733	21764	28.18	89.06

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ibuprofen**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20205-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ibuprofen; Ibuprofenum

Special notes

When selecting the *Ibuprofen* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ibuprofen	8	10	37

Second-stage model

For differentiation of the substance/substance group *Ibuprofen* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ibuprofen* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Tretinoin	95.43	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ibuprofen* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ibuprofen*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ibuprofen	11352219	20774	40	20120124
Caelo	Ibuprofen	172271	23641	40	20170831*
Caelo	Ibuprofen	19000539	25190	40	20200316*
Caelo	Ibuprofen	22003138	26484	40	20221020*
Euro OTC	Ibuprofen	1211011-02	21248	40	1501533
Euro OTC	Ibuprofen	1410025-02	23587	40	20141125
Euro OTC	Ibuprofen	2004027	25278	40	20200603*
Euro OTC	Ibuprofen	2208025	26339	40	20220915*
Euro OTC	Ibuprofen	2208025	26339SI	20	20220915*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 340 spectra of 9 reference samples from the substance/substance group *Ibuprofen*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 622 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 430 spectra of 12 reference samples from the substance/substance group *Ibuprofen*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ibuprofen	13105108	21321	40
Caelo	Ibuprofen	183003	24557	40
Caelo	Ibuprofen	22002352	26359	40
Caelo	Ibuprofen	22004099	26498	40
Caelo	Ibuprofen	23000201	26722	40
Euro OTC	Ibuprofen	2210019	26430	40
Euro OTC	Ibuprofen	2301018	26521	40
Euro OTC	Ibuprofen	2212017	26531	40
Euro OTC	Ibuprofen	2301054	26575	40
Fagron	Ibuprofen	23C20-B03-229831	26827	30
Caelo	Ibuprofen	22002352	26359SI	20
Caelo	Ibuprofen	22003138	26484SI†	20

- 201 654 spectra from a total of 4034 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 151 spectra from 76 *Apo-Ident* customers from 39 batches from the substance/substance group *Ibuprofen*.
- Among them are spectra of independent samples from 36 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ibuprofen	2210019-01	1
	Ibuprofen	2212017-01	1
	Ibuprofen	2301018-01	2
	Ibuprofen	2301054-01	2
Audor Pharma	Ibuprofen	2210019-01	5
Caelo	Ibuprofen		1
Caelo	Ibuprofen	1410025-02	1
Caelo	Ibuprofen	17227101	1
Caelo	Ibuprofen	17227102	1
Caelo	Ibuprofen	17351401	3
Caelo	Ibuprofen	17351403	1
Caelo	Ibuprofen	17351410	1
Caelo	Ibuprofen	183003002	1
Caelo	Ibuprofen	18300303	1
Caelo	Ibuprofen	18300304	2
Caelo	Ibuprofen	21000655001	1
Caelo	Ibuprofen	220002352001	1
Caelo	Ibuprofen	22003138003	1
Caelo	Ibuprofen	22003138004	1
Caelo	Ibuprofen	22003138006	1
Caelo	Ibuprofen	22004099001	1
Caelo	Ibuprofen	2208025-01	1
Caelo	Ibuprofen	2210019-01	1
Caesar & Loretz GmbH...	Ibuprofen	18300304	1
Caesar & Loretz GmbH...	Ibuprofen	183003002	1
Caesar & Loretz GmbH...	Ibuprofen	21000655003	1
Caesar & Loretz GmbH	Ibuprofen	183003002	1
Caesar & Loretz GmbH	Ibuprofen	21000655001	4
Caesar & Loretz GmbH	Ibuprofen	21000655004	1
Caesar & Loretz GmbH	Ibuprofen	22002352001	2
Caesar & Loretz GmbH	Ibuprofen	22003138004	2
Caesar & Loretz GmbH	Ibuprofen	22004099001	4
Caesar & Loretz GmbH	Ibuprofen	22004099003	1
Euro OTC	Ibuprofen	1211011-01	1
Euro OTC	Ibuprofen	1410025-01	6
Euro OTC	Ibuprofen	1410025-02	7
Euro OTC	Ibuprofen	2004027-01	2
Euro OTC	Ibuprofen	2004027-02	2
Euro OTC	Ibuprofen	2208025	1
Euro OTC	Ibuprofen	220802501	1
Euro OTC	Ibuprofen	2208025-01	30
Euro OTC	Ibuprofen	220825-01	1
Euro OTC	Ibuprofen	2210019-01	22
Euro OTC	Ibuprofen	2210019-02	7
Euro OTC	Ibuprofen	221201701	1
Euro OTC	Ibuprofen	2212017-01	1
Euro OTC	Ibuprofen	2301018-01	5
Euro OTC	Ibuprofen	7050-4896	2
Euro OTC	Ibuprofen	9061807	1
Euro/Sanacorp	Ibuprofen	2208025-01	2
Fagron	Ibuprofen	22K07-B12-224949	2
GEHE	Ibuprofen	15103011	1
GEHE	Ibuprofen	22003138004	1
Gehe	Ibuprofen	22003138008	3
Jenne	Ibuprofen	22003138003	2

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 235 916 spectra from 1515 *Apo-Ident* customers from a total of 49 219 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ibuprofen* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ibuprofen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	340	0	152 622
Type B	0	430	0	201 654
Type C	0	151	0	235 916

The substance/substance group *Ibuprofen* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2353 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6047 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 96.0265 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20774	26339	12.47	97.97
21248	21248	0.00	99.35
23587	25278	6.46	98.87
23641	23641	0.00	99.82
25190	25190	0.00	97.14
25278	25278	0.00	99.42
26339	26339	0.00	95.43
26484	26484	0.00	95.63

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Indometacin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20720-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Indometacin; Indometacinum

Special notes

When selecting the *Indometacin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Indometacin	6	4	33

Second-stage model

For differentiation of the substance/substance group *Indometacin* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Indometacin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Midazolam hydrochloride	114.41	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Indometacin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Indometacin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Indometacin	1012009-02	20720	40	1402050
Euro OTC	Indometacin	1205002-01	21327	40	20120521
Euro OTC	Indometacin	1512031	22291	60	20160122*
Euro OTC	Indometacin	1612017	22981	40	20170209*
Fagron	Indometacin	18H14-B04-365453	25062	40	20180920
Fagron	Indometacin	21E12-F04-379312	25841	50	20210811

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 270 spectra of 6 reference samples from the substance/substance group *Indometacin*. These

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 692 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 6 reference samples from the substance/substance group *Indometacin*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Indometacin	1801040	23969	40
Euro OTC	Indometacin	2106012	25762	40
Fagron	Indometacin	17I08-B06-339738	23715	40
Fagron	Indometacin	23C04-B10-230386	26896	30
Fagron	Indometacin	21E12-F04-379312	25841SI†	10
Fagron	Indometacin	23C04-B10-230386	26896SI	20

- 201 904 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 153 spectra from 75 *Apo-Ident* customers from 35 batches from the substance/substance group *Indometacin*.
- Among them are spectra of independent samples from 33 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Indometacin	2106012-01	1
	Indometacin	2106012-02	3
apo-ident	Indometacin	1801040-01	1
Caelo	Indometacin	1512031-01	1
Caelo	Indometacin	1801040-01	3
Caelo	Indometacin	1801040-02	1
Euro OTC	Indometacin	1202002-02	1
Euro OTC	Indometacin	1205002-01	2
Euro OTC	Indometacin	1205002-02	2
Euro OTC	Indometacin	1512031-01	17
Euro OTC	Indometacin	16110102	1
Euro OTC	Indometacin	161201-02	1
Euro OTC	Indometacin	1612017-01	9
Euro OTC	Indometacin	1612017-02	9
Euro OTC	Indometacin	1612017-2	1
Euro OTC	Indometacin	180104001	2
Euro OTC	Indometacin	1801040-01	25
Euro OTC	Indometacin	180104002	1
Euro OTC	Indometacin	1801040-02	19
Euro OTC	Indometacin	1801040-03	5
Euro OTC	Indometacin	1801044-02	1
Euro OTC	Indometacin	201606272030	1
Euro OTC	Indometacin	201612162018	2
Euro OTC	Indometacin	2091716	1
Euro OTC	Indometacin	2100012-01	1
Euro OTC	Indometacin	2106012-01	16
Euro OTC	Indometacin	2106012-12	1
Euro OTC	Indometacin	27101709	1
Euro OTC	Indometacin	612017-02	1
Euro/ Euro	Indometacin	1801040-01	1
Euro/Krieger	Indometacin	1801040-02	1
Fagron	Indometacin		1
Fagron	Indometacin	14I08-B06-343286	1
Fagron	Indometacin	14I25-B02-303648	1
Fagron	Indometacin	15L09-B08-315982	1
Fagron	Indometacin	17I08B06	1
Fagron	Indometacin	17I08-B06-339738	2
Fagron	Indometacin	17I08-B06-343286	1
Fagron	Indometacin	18H14-B03-352947	1
Fagron	Indometacin	18H14-B03-359139	1
Fagron	Indometacin	18H14-B04-368823	1
Gehe	Indometacin	1512031-01	1
Krieger/Euro	Indometacin	4932195	1
Noweda	Indometacin	1801040-01	3
Sanacorp	Indometacin	1612017-02	1
Sanacorp	Indometacin	1801040-03	1
Sanacorp	Indometacin	2106012-01	2
Sanacorp	Indometacin	2106012-02	1

- 235 914 spectra from 1515 *Apo-Ident* customers from a total of 49 224 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Indometacin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

all relevant spectra of the various substances were compared with *Indometacin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	270	0	152 692
Type B	0	180	0	201 904
Type C	0	152	1	235 914

The substance/substance group *Indometacin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7778 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9007 %)	99.3464 % (> 97.3856 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20720	20720	0.00	193.93
21327	20720	7.00	194.71
22291	22291	0.00	192.66
22981	22981	0.00	194.35
25062	22291	6.00	195.93
25841	22981	6.81	200.16

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Iodoform**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20094-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Iodoform; Iodoformium

Special notes

When selecting the *Iodoform* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Iodoform	7	8	166

Second-stage model

For differentiation of the substance/substance group *Iodoform* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Iodoform* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Menthol	197.45	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Iodoform* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Iodoform*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Iodoform	12283206	21297	40	20130709
Caelo	Iodoform	16012302	23192	40	AR-17-FG-012459-01
Caelo	Iodoform	16012302	23407	40	20160211
Caelo	Iodoform	191132	24710	40	20190524*
Caelo	Iodoform	21000186	25647	40	20210316*
Caelo	Iodoform	21000181	25648	40	20210330*
Caelo	Iodoform	22003551	26627	40	20230130*
Fagron	Iodoform	12L11-B41	21278	40	20140113

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 320 spectra of 8 reference samples from the substance/substance group *Iodoform*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 642 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 350 spectra of 11 reference samples from the substance/substance group *Iodoform*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Iodoform	170860	23652	30
Caelo	Iodoform	180919	24012	40
Caelo	Iodoform	182495	24380	40
Caelo	Iodoform	22000203	26020	40
Caelo	Iodoform	22000204	26021	40
Caelo	Iodoform	22003550	26628	40
Caelo	Iodoform	24000893	27238	40
Caelo	Iodoform	24000892	27263	40
Caelo	Iodoform	22000203	26020SI	10
Caelo	Iodoform	22000204	26021SI	10
Caelo	Iodoform	22003551	26627SI†	20

- 201 734 spectra from a total of 4036 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 783 spectra from 302 *Apo-Ident* customers from 169 batches from the substance/substance group *Iodoform*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 166 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Iodoform	22000203005	1
	Iodoform	22000203006	3
	Iodoform	22000204001	2
	Iodoform	22003550002	1
	Iodoform	22003550003	1
	Iodoform	22003551002	1
	Iodoform	22003551003	1
	Iodoform	22003607002	2
	Iodoform	22003607003	1
AHC	Iodoform	22003550003	1
AHC	Iodoform	22003551002	1
AHC	Iodoform	22003551005	1
AHD	Iodoform	22000204001	2
AHD	Iodoform	22003551002	2
AHD	Iodoform	22003607002	1
cae	Iodoform	191132003	1
Caelo	Iodoform	1010316	1
Caelo	Iodoform	10320407	1
Caelo	Iodoform	12070102	2
Caelo	Iodoform	12070105	1
Caelo	Iodoform	12070303	2
Caelo	Iodoform	12070407	1
Caelo	Iodoform	12070501	1
Caelo	Iodoform	12070502	1
Caelo	Iodoform	12070601	4
Caelo	Iodoform	12070602	3
Caelo	Iodoform	12070605	1
Caelo	Iodoform	12070606	2
Caelo	Iodoform	12070608	3
Caelo	Iodoform	12150902	6
Caelo	Iodoform	12150903	1
Caelo	Iodoform	12150905	3
Caelo	Iodoform	12150907	1
Caelo	Iodoform	12150908	4
Caelo	Iodoform	12150910	6
Caelo	Iodoform	12283201	3
Caelo	Iodoform	12283202	5
Caelo	Iodoform	12283206	3
Caelo	Iodoform	12283303	2
Caelo	Iodoform	12283304	1
Caelo	Iodoform	12283307	1
Caelo	Iodoform	14077601	1
Caelo	Iodoform	14077602	1
Caelo	Iodoform	14077603	2
Caelo	Iodoform	14077606	2
Caelo	Iodoform	14077607	1
Caelo	Iodoform	14077702	7
Caelo	Iodoform	14229504	2
Caelo	Iodoform	14229505	1
Caelo	Iodoform	14229507	3
Caelo	Iodoform	14229508	2
Caelo	Iodoform	14230001	6
Caelo	Iodoform	14230002	3
Caelo	Iodoform	14230003	1
Caelo	Iodoform	14230006	5
Caelo	Iodoform	14230007	3
Caelo	Iodoform	14230008	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Iodoform	14230302	2
Caelo	Iodoform	14230304	2
Caelo	Iodoform	14230305	9
Caelo	Iodoform	14230306	6
Caelo	Iodoform	14230308	6
Caelo	Iodoform	1527104	1
Caelo	Iodoform	15276001	3
Caelo	Iodoform	15276002	6
Caelo	Iodoform	15276101	6
Caelo	Iodoform	15276102	5
Caelo	Iodoform	15276103	5
Caelo	Iodoform	15276104	4
Caelo	Iodoform	15276105	8
Caelo	Iodoform	15276107	1
Caelo	Iodoform	15276108	3
Caelo	Iodoform	15276109	3
Caelo	Iodoform	1527611	1
Caelo	Iodoform	15276111	6
Caelo	Iodoform	15276113	1
Caelo	Iodoform	1576103	1
Caelo	Iodoform	16012201	10
Caelo	Iodoform	16012202	2
Caelo	Iodoform	16012204	6
Caelo	Iodoform	16012205	2
Caelo	Iodoform	16012206	6
Caelo	Iodoform	16012207	7
Caelo	Iodoform	16012210	6
Caelo	Iodoform	16012302	5
Caelo	Iodoform	16012305	6
Caelo	Iodoform	16012306	8
Caelo	Iodoform	16012308	3
Caelo	Iodoform	16012309	5
Caelo	Iodoform	16012311	1
Caelo	Iodoform	17086001	6
Caelo	Iodoform	17086002	4
Caelo	Iodoform	17086003	5
Caelo	Iodoform	17086004	10
Caelo	Iodoform	17086005	10
Caelo	Iodoform	17086006	12
Caelo	Iodoform	17086008	3
Caelo	Iodoform	17086012	3
Caelo	Iodoform	17086066	1
Caelo	Iodoform	18041821	1
Caelo	Iodoform	18091801	1
Caelo	Iodoform	18091802	7
Caelo	Iodoform	18091803	1
Caelo	Iodoform	18091804	4
Caelo	Iodoform	18091805	17
Caelo	Iodoform	18091806	10
Caelo	Iodoform	18091807	2
Caelo	Iodoform	18091902	1
Caelo	Iodoform	18091904	1
Caelo	Iodoform	18091905	16
Caelo	Iodoform	18091906	4
Caelo	Iodoform	18091907	2
Caelo	Iodoform	18091909	4
Caelo	Iodoform	18091911	4
Caelo	Iodoform	18091912	6
Caelo	Iodoform	18091912P-200326-10	1
Caelo	Iodoform	18249501	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Iodoform	18249502	11
Caelo	Iodoform	18249503	6
Caelo	Iodoform	1911320004	1
Caelo	Iodoform	191132001	13
Caelo	Iodoform	191132002	9
Caelo	Iodoform	191132004	19
Caelo	Iodoform	191132005	6
Caelo	Iodoform	19113201	14
Caelo	Iodoform	19113204	2
Caelo	Iodoform	1961132001	1
Caelo	Iodoform	1961132004	1
Caelo	Iodoform	20000241001	17
Caelo	Iodoform	20000241004	4
Caelo	Iodoform	20000241005	5
Caelo	Iodoform	20000241006	12
Caelo	Iodoform	20000241007	1
Caelo	Iodoform	20000241008	12
Caelo	Iodoform	20000241009	1
Caelo	Iodoform	21000181003	7
Caelo	Iodoform	21000181004	3
Caelo	Iodoform	21000186001	9
Caelo	Iodoform	21000186002	15
Caelo	Iodoform	21000186003	3
Caelo	Iodoform	21000186006	8
Caelo	Iodoform	21000186007	1
Caelo	Iodoform	21000186009	1
Caelo	Iodoform	21000191003	1
Caelo	Iodoform	2100186006	1
Caelo	Iodoform	21051305	1
Caelo	Iodoform	22000203001	3
Caelo	Iodoform	22000203006	1
Caelo	Iodoform	22000204001	1
Caelo	Iodoform	22000204002	2
Caelo	Iodoform	22000204004	1
Caelo	Iodoform	22003607002	4
Caelo	Iodoform	22003607003	1
Caelo	Iodoform	220127	1
Caelo	Iodoform	23021715	1
Caelo	Iodoform	28011503	1
Caelo	Iodoform	3041407	1
Caelo	Iodoform	320E01726	1
Caelo	Iodoform	46(18091805)	1
Caelo	Iodoform	47(18091905)	1
Caelo	Iodoform	48(18091905)	1
Caelo	Iodoform	49(18091911)	1
Caelo	Iodoform	52(20000241001)	1
Caelo	Iodoform	53(20000241001)	1
Caelo	Iodoform	54(20000241008)	2
Caelo	Iodoform	55(20000241001)	1
Caeolo/Sanacorp	Iodoform	21000181003	1
Caesar & Loretz GmbH...	Iodoform	21000181003	4
Caesar & Loretz GmbH...	Iodoform	18091906	1
Caesar & Loretz GmbH...	Iodoform	18249502	1
Caesar & Loretz GmbH...	Iodoform	12070501	3
Caesar & Loretz GmbH...	Iodoform	191132001	2
Caesar & Loretz GmbH...	Iodoform	19113201	1
Caesar & Loretz GmbH...	Iodoform	21000186001	1
Caesar & Loretz GmbH...	Iodoform	191132001	1
Caesar & Loretz GmbH/Gehe	Iodoform	21000186001	1
Caesar & Loretz GmbH/GEHE	Iodoform	21000186001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Iodoform	191132001	4
Caesar & Loretz GmbH...	Iodoform	191132004	1
Caesar & Loretz GmbH...	Iodoform	21000186003	1
Caesar & Loretz GmbH...	Iodoform	AP220630-03	1
Caesar & Loretz GmbH...	Iodoform	AP221112-01	1
Caesar & Loretz GmbH...	Iodoform	21000186003	1
Caesar & Loretz GmbH...	Iodoform	18249502	1
Caesar & Loretz GmbH...	Iodoform	191132001	1
Caesar & Loretz GmbH...	Iodoform	19113203	1
Caesar & Loretz GmbH...	Iodoform	19113204	1
Caesar & Loretz GmbH...	Iodoform	20000241002	2
Caesar & Loretz GmbH...	Iodoform	20000241004	1
Caesar & Loretz GmbH...	Iodoform	AP220812-01	2
Caesar & Loretz GmbH	Iodoform	12150907	1
Caesar & Loretz GmbH	Iodoform	18091902	2
Caesar & Loretz GmbH	Iodoform	18091905	4
Caesar & Loretz GmbH	Iodoform	18091906	1
Caesar & Loretz GmbH	Iodoform	18091909	1
Caesar & Loretz GmbH	Iodoform	18091911	1
Caesar & Loretz GmbH	Iodoform	18091912	1
Caesar & Loretz GmbH	Iodoform	18249502	8
Caesar & Loretz GmbH	Iodoform	191132001	6
Caesar & Loretz GmbH	Iodoform	191132002	1
Caesar & Loretz GmbH	Iodoform	191132004	3
Caesar & Loretz GmbH	Iodoform	191132005	2
Caesar & Loretz GmbH	Iodoform	19113201	6
Caesar & Loretz GmbH	Iodoform	19113203	1
Caesar & Loretz GmbH	Iodoform	19113204	1
Caesar & Loretz GmbH	Iodoform	20000241001	4
Caesar & Loretz GmbH	Iodoform	20000241005	3
Caesar & Loretz GmbH	Iodoform	20000241006	2
Caesar & Loretz GmbH	Iodoform	20000241008	5
Caesar & Loretz GmbH	Iodoform	20000241009	1
Caesar & Loretz GmbH	Iodoform	21000181003	4
Caesar & Loretz GmbH	Iodoform	21000186001	1
Caesar & Loretz GmbH	Iodoform	21000186002	5
Caesar & Loretz GmbH	Iodoform	21000186003	4
Caesar & Loretz GmbH	Iodoform	21000186004	1
Caesar & Loretz GmbH	Iodoform	21000186006	1
Caesar & Loretz GmbH	Iodoform	21000186007	2
Caesar & Loretz GmbH	Iodoform	22000203001	1
Caesar & Loretz GmbH	Iodoform	22000204002	1
Caesar & Loretz GmbH	Iodoform	22003607002	1
Caesar & Loretz GmbHGehe	Iodoform	18249502	1
Caesar & Loretz Hilden	Iodoform	18091905	2
Caesar Loretz	Iodoform	20000241001	1
Caesar u.Loretz	Iodoform	16012209	2
Cao	Iodoform	18249503	1
Cesar&Loretz GmbH Noweda	Iodoform	19113201	1
Euro OTC	Iodoform	14229504	2
Fagron	Iodoform	12E30-N01	2
Fagron	Iodoform	12L11-B41	1
Fagron	Iodoform	12L11-B41-290055	1
Fagron	Iodoform	14229508	1
Fagron	Iodoform	14D09-B14-293029	1
Fagron	Iodoform	16012302	1
Fagron	Iodoform	18091803	1
Fiebig	Iodoform	16012206	1
fragon	Iodoform	12283303	1
Gehe	Iodoform	14230008	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Iodoform	17086001	1
GEHE	Iodoform	17086002	1
GEHE	Iodoform	17086003	1
Gehe	Iodoform	191132001	1
Gehe	Iodoform	22003551003	1
Henry Lamotte Oils G…	Iodoform	16012309	1
Kehr	Iodoform	22003607003	1
Midas	Iodoform	16012306	1
Nachprüfung von Juni 2018	Iodoform	15276103	1
Noweda /Cealo	Iodoform	20000241005	1
Noweda	Iodoform	10320402	1
Noweda	Iodoform	12070407	1
Noweda	Iodoform	17086012	1
Noweda	Iodoform	18091805	1
Noweda	Iodoform	18091806	1
Noweda	Iodoform	18091902	1
Noweda	Iodoform	19113201	1
Noweda	Iodoform	20000241008	2
Noweda	Iodoform	21000186002	1
Noweda	Iodoform	22000204001	1
Phoenix	Iodoform	12070601	1
Phoenix	Iodoform	191132001	1
Phoenix	Iodoform	22003607003	1
phönix	Iodoform	18249502	2
Sanacorp	Iodoform	17086005	1
Sanacorp	Iodoform	18091805	1
Sanacorp	Iodoform	22003551002	1
Sanacorp	Iodoform	22003607003	2

- 235 284 spectra from 1515 *Apo-Ident* customers from a total of 49 091 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Iodoform* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Iodoform* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	350	0	201 734
Type C	0	777	6	235 284

The substance/substance group *Iodoform* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.2857 %)
Type C	100.0000 % (> 99.9007 %)	99.2337 % (> 98.8506 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21278	23192	20.90	233.61
21297	26627	28.89	228.92
23192	23192	0.00	241.72
23407	23192	13.59	239.05
24710	24710	0.00	243.64
25647	25647	0.00	243.85
25648	25648	0.00	242.29
26627	26627	0.00	233.22

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ipratropium bromide**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20911-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ipratropium bromide; Ipratropii bromidum

Special notes

When selecting the *Ipratropium bromide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ipratropium bromide	5	3	12

Second-stage model

For differentiation of the substance/substance group *Ipratropium bromide* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ipratropium bromide* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	133.18	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ipratropium bromide* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ipratropium bromide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ipratropium bromide	12C15-N01	20911	40	1403675
Fagron	Ipratropium bromide	12K01-N08	21272	40	20121025
Fagron	Ipratropium bromide	18H30-B09-359179	24947	40	20180918
Fagron	Ipratropium bromide	21E27-B06-213614	25903	40	20210908
Fagron	Ipratropium bromide	23C07-B08-230203	26897	40	20230418

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Ipratropium bromide*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.
- 152 762 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 5 reference samples from the substance/substance group *Ipratropium bromide*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ipratropium bromide	15C04-B02-321674	22747	40
Fagron	Ipratropium bromide	16K07-B05-335330	23597	40
Fagron	Ipratropium bromide	18B19-B05-346997	23992	40
Fagron	Ipratropium bromide	21E27-B06-213614	25903SI†	10
Fagron	Ipratropium bromide	23C07-B08-230203	26897SI†	20

- 201 934 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 27 spectra from 15 *Apo-Ident* customers from 13 batches from the substance/substance group *Ipratropium bromide*.
- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ipratropium bromide	21E27-B06-213614	1
Euro OTC	Ipratropium bromide	18B19-B05-348556	1
Fagron	Ipratropium bromide	14B05-B16-294566	1
Fagron	Ipratropium bromide	15C04-B02-321674	1
Fagron	Ipratropium bromide	18B19-B05-348556	2
Fagron	Ipratropium bromide	18B19-B05-356276	8
Fagron	Ipratropium bromide	18H30-B09-359170	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Ipratropium bromide	18H30-B09-367187/1850002262	1
Fagron	Ipratropium bromide	21A14-F02	2
Fagron	Ipratropium bromide	21A14-F02377074	1
Fagron	Ipratropium bromide	21A14-F02-377075	2
Fagron	Ipratropium bromide	21E27-B06-213614	3
Fagron	Ipratropium bromide	F02-3770705	1
Fargon	Ipratropium bromide	18B19-B055-356276	1
Fragon	Ipratropium bromide	2050002969	1

- 236 040 spectra from 1515 *Apo-Ident* customers from a total of 49 246 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ipratropium bromide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ipratropium bromide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	150	0	201 934
Type C	0	27	0	236 040

The substance/substance group *Ipratropium bromide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 77.7778 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20911	20911	0.00	189.46
21272	20911	7.81	189.88
24947	20911	16.98	193.18
25903	20911	23.60	191.78
26897	20911	15.46	188.97

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Isoleucine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21045-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Isoleucine; Isoleucinum; L-isoleucine

Special notes

When selecting the *Isoleucine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Isoleucine	7	14	16

Second-stage model

For differentiation of the substance/substance group *Isoleucine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Isoleucine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Leucine	62.74	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Isoleucine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Isoleucine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Isoleucine	1604057	22566	40	20160601*
Euro OTC	Isoleucine	1704022	23386	40	20170612*
Euro OTC	Isoleucine	1909025	24931	40	20191015*
Euro OTC	Isoleucine	2301011	26534	40	20230201*
Euro OTC	Isoleucine	2301011	26534SI	20	20230201*
Fagron	Isoleucine	13E02-B01-286930	21045	40	1403154
Fagron	Isoleucine	13E02-B01	21332	40	20130621
Fagron	Isoleucine	20B12-B01-197402	25441	40	20200313

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 300 spectra of 8 reference samples from the substance/substance group *Isoleucine*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 662 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 620 spectra of 17 reference samples from the substance/substance group *Isoleucine*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Isoleucine	1611007	22869	40
Euro OTC	Isoleucine	1708027	23702	40
Euro OTC	Isoleucine	1711034	23869	40
Euro OTC	Isoleucine	1803019	24080	40
Euro OTC	Isoleucine	1805013	24115	40
Euro OTC	Isoleucine	1901010	24515	40
Euro OTC	Isoleucine	2101041	25530	40
Euro OTC	Isoleucine	2111017	25891	50
Euro OTC	Isoleucine	2309020	27011	40
Euro OTC	Isoleucine	2404003	27288	40
Fagron	Isoleucine	21B01-B06-210568	26292	40
Fagron	Isoleucine	22G01-B04-221842	26682	40
Fagron	Isoleucine	23C07-B07-230992	27043	40
Fagron	Isoleucine	24A10-B08-235292	27425	40
Euro OTC	Isoleucine	2111017	25891SI	10
Fagron	Isoleucine	21B01-B06-210568	26292SI	20
Fagron	Isoleucine	22G01-B04-221842	26682SI	20

- 201 464 spectra from a total of 4031 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 32 spectra from 12 *Apo-Ident* customers from 17 batches from the substance/substance group *Isoleucine*.

- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Isoleucine	2111017-01	2
Euro OTC	Isoleucine	1704022-01	1
Euro OTC	Isoleucine	1708027-01	1
Euro OTC	Isoleucine	1711034-01	1
Euro OTC	Isoleucine	1805013-02	1
Euro OTC	Isoleucine	1901010-01	1
Euro OTC	Isoleucine	2006027-01	5
Euro OTC	Isoleucine	2101041-01	1
Euro OTC	Isoleucine	2111017-01	3
Fagro WE:19.05.16 EK...	Isoleucine	15A14-B09-314881	1
Fagron	Isoleucine	12080167	1
Fagron	Isoleucine	13A22-N03	1
Fagron	Isoleucine	13E02-B01-286930	1
Fagron	Isoleucine	14D08-B02-296089	2
Fagron	Isoleucine	16H24-B03-331739	1
Fagron	Isoleucine	17010483	2
Fagron	Isoleucine	17H14-B04-339008	5
Sanacorp	Isoleucine	17H14-B04-339008	1
Synop WE:18.12.17 E...	Isoleucine	17H14-B04-339009	1

- 236 035 spectra from 1515 *Apo-Ident* customers from a total of 49 241 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Isoleucine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Isoleucine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	620	0	201 464
Type C	0	32	0	236 035

The substance/substance group *Isoleucine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0323 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 81.2500 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21045	21045	0.00	102.70
21332	21045	4.84	102.24
22566	22566	0.00	106.57
23386	23386	0.00	107.27
24931	24931	0.00	105.05
25441	26534	5.12	109.58
26534	26534	0.00	106.23

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Isosorbide dinitrate 40%**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20213-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Isosorbide dinitrate 40%; Isorbidi dinitras 40%

Special notes

When selecting the *Isosorbide dinitrate 40%* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Isosorbide dinitrate 40%	5	3	229

Second-stage model

For differentiation of the substance/substance group *Isosorbide dinitrate 40%* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Isosorbide dinitrate 40%* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	65.40	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Isosorbide dinitrate 40%* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Isosorbide dinitrate 40%*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Isosorbide dinitrate 40%	12F08-N04	20891	40	20120801
Fagron	Isosorbide dinitrate 40%	13D15-N02	21347	39	20130410
Fagron	Isosorbide dinitrate 40%	15I10-B01-328577	23200	40	1709092
Fagron	Isosorbide dinitrate 40%	15I10-B01-328577	23598	30	20150922
Fagron	Isosorbide dinitrate 40%	17C29-B01-339447	24057	40	20170517
Fagron	Isosorbide dinitrate 40%	23F19-B04-231383	27044	40	20231004

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 229 spectra of 6 reference samples from the substance/substance group *Isosorbide dinitrate 40%*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.
- 152 733 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 5 reference samples from the substance/substance group *Isosorbide dinitrate 40%*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Isosorbide dinitrate 40%	15I10-B01-315217	22762	40
Fagron	Isosorbide dinitrate 40%	18J18-B01-363845	25065	40
Fagron	Isosorbide dinitrate 40%	22D11-B05-215487	26300	40
Fagron	Isosorbide dinitrate 40%	22D11-B05-215487	26300SI	10
Fagron	Isosorbide dinitrate 40%	23F19-B04-231383	27044SI†	20

- 201 934 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1054 spectra from 437 *Apo-Ident* customers from 269 batches from the substance/substance group *Isosorbide dinitrate 40%*.
- Among them are spectra of independent samples from 227 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Isosorbide dinitrate 40%		1
	Isosorbide dinitrate 40%	17c29-b01-348859	1
	Isosorbide dinitrate 40%	2203089	4
	Isosorbide dinitrate 40%	22D11-B05-215487	1
	Isosorbide dinitrate 40%	22D11-B05-216314	7

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
	Isosorbide dinitrate 40%	22D11-B05-225756	2
	Isosorbide dinitrate 40%	22D11-b05225757	1
	Isosorbide dinitrate 40%	22D11-B05-225757	1
	Isosorbide dinitrate 40%	22D11B05229443	1
	Isosorbide dinitrate 40%	22D11-B05-229443	2
	Isosorbide dinitrate 40%	23F19-B04-231383	1
	Isosorbide dinitrate 40%	B0521631004	1
AEP GmbH	Isosorbide dinitrate 40%	B01-3638405	1
AHD 09.03.2015	Isosorbide dinitrate 40%	14D09-B03-294281	1
AHD	Isosorbide dinitrate 40%	17C29-B01-350470	1
Ahd	Isosorbide dinitrate 40%	2203089	1
AHD	Isosorbide dinitrate 40%	22D11-B05-225757	5
AHD	Isosorbide dinitrate 40%	23F19-B04-231383	1
Alliance / Fargon	Isosorbide dinitrate 40%	18J18-B01-359177	2
Allianz Healthcare 1...	Isosorbide dinitrate 40%	14D09-B03-300234	1
Anzag	Isosorbide dinitrate 40%	12C08-N05	2
Anzag	Isosorbide dinitrate 40%	15/10-B01-328577	1
Anzag	Isosorbide dinitrate 40%	1510B01315217	1
Anzah / Henry lammotte	Isosorbide dinitrate 40%	14D09-B03-294281	2
apo-ident	Isosorbide dinitrate 40%	18J18-B01-359177	1
Avara Shannon / Eber...	Isosorbide dinitrate 40%	193469	2
Avara Shannon Pharm ...	Isosorbide dinitrate 40%	195293	1
Avara Shannon Pharm....	Isosorbide dinitrate 40%	18J18-B01-358247	1
Avara Shannon Pharm/ gehe	Isosorbide dinitrate 40%	195293	1
Avara Shannon	Isosorbide dinitrate 40%		1
Caelo	Isosorbide dinitrate 40%		1
Caelo	Isosorbide dinitrate 40%	11/17-N05	1
Caelo	Isosorbide dinitrate 40%	11D12-N01	1
Caelo	Isosorbide dinitrate 40%	13/26-N18	1
Caelo	Isosorbide dinitrate 40%	13D15-N02	3
Caelo	Isosorbide dinitrate 40%	13F27-N04	1
Caelo	Isosorbide dinitrate 40%	149168	2
Caelo	Isosorbide dinitrate 40%	14D09B03294281	1
Caelo	Isosorbide dinitrate 40%	14D-09-B03-300234	1
Caelo	Isosorbide dinitrate 40%	14D09-B03-307018	1
Caelo	Isosorbide dinitrate 40%	14D09-B03-308419	4
Caelo	Isosorbide dinitrate 40%	15/10-B01-320081	4
Caelo	Isosorbide dinitrate 40%	15/10-B01-325474	2
Caelo	Isosorbide dinitrate 40%	15/10-B01-328577	1
Caelo	Isosorbide dinitrate 40%	15/10-B01-331286	1
Caelo	Isosorbide dinitrate 40%	1510-B01-315217	1
Caelo	Isosorbide dinitrate 40%	1510-B01-320081	2
Caelo	Isosorbide dinitrate 40%	15-10b01-328132	1
Caelo	Isosorbide dinitrate 40%	15-10-b01-328132	2
Caelo	Isosorbide dinitrate 40%	1510b1320782	1
Caelo	Isosorbide dinitrate 40%	15I10-B01	1
Caelo	Isosorbide dinitrate 40%	15I10-B01-328577	1
Caelo	Isosorbide dinitrate 40%	15l10-B01-325474	1
Caelo	Isosorbide dinitrate 40%	17C29-B01-335070	2
Caelo	Isosorbide dinitrate 40%	17C29-B01-335071	1
Caelo	Isosorbide dinitrate 40%	17c29-B01-339447	1
Caelo	Isosorbide dinitrate 40%	17C29B01339447	1
Caelo	Isosorbide dinitrate 40%	17C29-B01-339447	2
Caelo	Isosorbide dinitrate 40%	17c29-b01-339448	1
Caelo	Isosorbide dinitrate 40%	17C29-B01-347248	1
Caelo	Isosorbide dinitrate 40%	17C29-B01-347589	3
Caelo	Isosorbide dinitrate 40%	17c29-b01-347885	4
Caelo	Isosorbide dinitrate 40%	17C29-B01-348859	2
Caelo	Isosorbide dinitrate 40%	17C29-B01-348860	1
Caelo	Isosorbide dinitrate 40%	17C29-B01-353161	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Isosorbide dinitrate 40%	18j18-b01-358247	1
Caelo	Isosorbide dinitrate 40%	18J18-B01-363844	1
Caelo	Isosorbide dinitrate 40%	18J18-B01-363845	1
Caelo	Isosorbide dinitrate 40%	18J18-B01-373438	1
Caelo	Isosorbide dinitrate 40%	193469	1
Caelo	Isosorbide dinitrate 40%	195293	1
Caelo	Isosorbide dinitrate 40%	701310-0001	1
Caelo	Isosorbide dinitrate 40%	701319-0003	1
ebe a	Isosorbide dinitrate 40%	14D09-B03-294281	1
Ebert-Jacobi	Isosorbide dinitrate 40%	15I10-B01-328132	1
Euro OTC	Isosorbide dinitrate 40%		1
Euro OTC	Isosorbide dinitrate 40%	13126-N18	1
Euro OTC	Isosorbide dinitrate 40%	15I10-B01325474	1
Euro OTC	Isosorbide dinitrate 40%	22D11-B05-215487	1
Fagro/Noweda	Isosorbide dinitrate 40%	17C29-B01-335070	1
Fagron	Isosorbide dinitrate 40%		9
Fagron	Isosorbide dinitrate 40%	10029-N10	1
Fagron	Isosorbide dinitrate 40%	101652	6
Fagron	Isosorbide dinitrate 40%	10-B01-320081	1
Fagron	Isosorbide dinitrate 40%	10C19-N01	1
Fagron	Isosorbide dinitrate 40%	10D29-N10	1
Fagron	Isosorbide dinitrate 40%	11/17-N05	1
Fagron	Isosorbide dinitrate 40%	11/17-No5	1
Fagron	Isosorbide dinitrate 40%	11D12-N01	2
Fagron	Isosorbide dinitrate 40%	11F28-N05	2
Fagron	Isosorbide dinitrate 40%	11I17-N05	1
Fagron	Isosorbide dinitrate 40%	11J17-N05	3
Fagron	Isosorbide dinitrate 40%	11l17-N05	1
Fagron	Isosorbide dinitrate 40%	1216M-03516	1
Fagron	Isosorbide dinitrate 40%	12C08-N05	2
Fagron	Isosorbide dinitrate 40%	12f08-n04	1
Fagron	Isosorbide dinitrate 40%	12F08-N04	8
Fagron	Isosorbide dinitrate 40%	12k14-n02	1
Fagron	Isosorbide dinitrate 40%	12K14N02	1
Fagron	Isosorbide dinitrate 40%	12K14-N02	6
Fagron	Isosorbide dinitrate 40%	13/26-N18	1
Fagron	Isosorbide dinitrate 40%	1309210009	1
Fagron	Isosorbide dinitrate 40%	1-36384005	1
Fagron	Isosorbide dinitrate 40%	1373438	1
Fagron	Isosorbide dinitrate 40%	13A07-0003	1
Fagron	Isosorbide dinitrate 40%	13A07-N13	7
Fagron	Isosorbide dinitrate 40%	13d15-n02	1
Fagron	Isosorbide dinitrate 40%	13D15-N02	7
Fagron	Isosorbide dinitrate 40%	13F27-N04	6
Fagron	Isosorbide dinitrate 40%	13F27-N040234/1300	1
Fagron	Isosorbide dinitrate 40%	13I26-N18	10
Fagron	Isosorbide dinitrate 40%	149168	11
Fagron	Isosorbide dinitrate 40%	14D09-B03	9
Fagron	Isosorbide dinitrate 40%	14D09-B03_294280	1
Fagron	Isosorbide dinitrate 40%	14D09-B03_294282	1
Fagron	Isosorbide dinitrate 40%	14D09-B03_308419	1
Fagron	Isosorbide dinitrate 40%	14D09-B03-294280	9
Fagron	Isosorbide dinitrate 40%	14D09B03294281	1
Fagron	Isosorbide dinitrate 40%	14D09-B03-294281	4
Fagron	Isosorbide dinitrate 40%	14D09-B03-294282	5
Fagron	Isosorbide dinitrate 40%	14D09-B03-294282Eber	1
Fagron	Isosorbide dinitrate 40%	14D09-B03-29481	1
Fagron	Isosorbide dinitrate 40%	14D09-B03-300234	14
Fagron	Isosorbide dinitrate 40%	14-D09-B03-300234	1
Fagron	Isosorbide dinitrate 40%	14D09B03300235	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Isosorbide dinitrate 40%	14D09-B03-300235	1
Fagron	Isosorbide dinitrate 40%	14D09-B03-305633	1
Fagron	Isosorbide dinitrate 40%	14D09-B03-307018	1
Fagron	Isosorbide dinitrate 40%	14D09-B03-308419	17
Fagron	Isosorbide dinitrate 40%	14d09-b03-313566	1
Fagron	Isosorbide dinitrate 40%	14D09-B03-313566	3
Fagron	Isosorbide dinitrate 40%	14D09-B3-308419	1
Fagron	Isosorbide dinitrate 40%	15/10B01-315217	1
Fagron	Isosorbide dinitrate 40%	15/10-B01-315217	8
Fagron	Isosorbide dinitrate 40%	15/10-B01-318522	1
Fagron	Isosorbide dinitrate 40%	15/10-B01-3200782	1
Fagron	Isosorbide dinitrate 40%	15/10-B01-320081	12
Fagron	Isosorbide dinitrate 40%	15/10-B01-320782	1
Fagron	Isosorbide dinitrate 40%	15/10-B01-325474	5
Fagron	Isosorbide dinitrate 40%	15/10-b01-328132	3
Fagron	Isosorbide dinitrate 40%	15/10-B01-328132	2
Fagron	Isosorbide dinitrate 40%	15/10-B01-328577	9
Fagron	Isosorbide dinitrate 40%	15/10-B01-331286	5
Fagron	Isosorbide dinitrate 40%	15/10-b01-331287	3
Fagron	Isosorbide dinitrate 40%	15/10-B01-331287	1
Fagron	Isosorbide dinitrate 40%	15/10-B10-331286	1
Fagron	Isosorbide dinitrate 40%	15/10-B01-325474	1
Fagron	Isosorbide dinitrate 40%	1510-B01-315217	2
Fagron	Isosorbide dinitrate 40%	15-10-b01-318522	1
Fagron	Isosorbide dinitrate 40%	1510B01320081	1
Fagron	Isosorbide dinitrate 40%	1510-B01320081	1
Fagron	Isosorbide dinitrate 40%	1510-B01-320081	1
Fagron	Isosorbide dinitrate 40%	1510B01325474	2
Fagron	Isosorbide dinitrate 40%	1510-B01-325474	1
Fagron	Isosorbide dinitrate 40%	1510-b01-325475	3
Fagron	Isosorbide dinitrate 40%	15-10-b01-325475	1
Fagron	Isosorbide dinitrate 40%	1510-b01-328132	1
Fagron	Isosorbide dinitrate 40%	1510B01328577	1
Fagron	Isosorbide dinitrate 40%	1510-B01-328577	2
Fagron	Isosorbide dinitrate 40%	15-10-b01-331287	5
Fagron	Isosorbide dinitrate 40%	151-b01-328132	2
Fagron	Isosorbide dinitrate 40%	15I10-B01	9
Fagron	Isosorbide dinitrate 40%	15I10-B01-310081	1
Fagron	Isosorbide dinitrate 40%	15I10-B01-315217	2
Fagron	Isosorbide dinitrate 40%	15I10-B01-318522	2
Fagron	Isosorbide dinitrate 40%	15I10-B01-320081	5
Fagron	Isosorbide dinitrate 40%	15I10-B01-320782	2
Fagron	Isosorbide dinitrate 40%	15I10-B01-325474	7
Fagron	Isosorbide dinitrate 40%	15I10-B01-328132	1
Fagron	Isosorbide dinitrate 40%	15I10-B01-328577	5
Fagron	Isosorbide dinitrate 40%	15I10B01331286	1
Fagron	Isosorbide dinitrate 40%	15I10-B01-331286	3
Fagron	Isosorbide dinitrate 40%	15l10-B01-320081	1
Fagron	Isosorbide dinitrate 40%	15l10-B01-325474	1
Fagron	Isosorbide dinitrate 40%	15L10B01325474	1
Fagron	Isosorbide dinitrate 40%	15l10-B01-328577	1
Fagron	Isosorbide dinitrate 40%	15l10-B01-331286	1
Fagron	Isosorbide dinitrate 40%	160629I	1
Fagron	Isosorbide dinitrate 40%	17C26-B01-347885	1
Fagron	Isosorbide dinitrate 40%	17C29_B01_350469	1
Fagron	Isosorbide dinitrate 40%	17C29-801-347885	1
Fagron	Isosorbide dinitrate 40%	17c29-b01	1
Fagron	Isosorbide dinitrate 40%	17C29-B01	14
Fagron	Isosorbide dinitrate 40%	17C29-B01_339447	1
Fagron	Isosorbide dinitrate 40%	17C29-B01_350469	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Isosorbide dinitrate 40%	17c29b01335070	1
Fagron	Isosorbide dinitrate 40%	17c29-b01-335070	2
Fagron	Isosorbide dinitrate 40%	17C29B01335070	1
Fagron	Isosorbide dinitrate 40%	17C29-B01335070	1
Fagron	Isosorbide dinitrate 40%	17C29-B01-335070	18
Fagron	Isosorbide dinitrate 40%	17c29-b01-335071	6
Fagron	Isosorbide dinitrate 40%	17C29-B01-335071	3
Fagron	Isosorbide dinitrate 40%	17C29B01339447	1
Fagron	Isosorbide dinitrate 40%	17C29-B01-339447	19
Fagron	Isosorbide dinitrate 40%	17c29-b01-339448	1
Fagron	Isosorbide dinitrate 40%	17C29-b01-339448	1
Fagron	Isosorbide dinitrate 40%	17C29-B01-339448	4
Fagron	Isosorbide dinitrate 40%	17C29-B01-346333	1
Fagron	Isosorbide dinitrate 40%	17C29-B01-347248	4
Fagron	Isosorbide dinitrate 40%	17C29B01347589	1
Fagron	Isosorbide dinitrate 40%	17C29-B01-347589	16
Fagron	Isosorbide dinitrate 40%	17C29-B01-347885	1
Fagron	Isosorbide dinitrate 40%	17c29-b01-348859	3
Fagron	Isosorbide dinitrate 40%	17C29B01348859	1
Fagron	Isosorbide dinitrate 40%	17C29-B01-348859	22
Fagron	Isosorbide dinitrate 40%	17C29-B01-348860	2
Fagron	Isosorbide dinitrate 40%	17C29-B01-34889	1
Fagron	Isosorbide dinitrate 40%	17c29-b01-350469	1
Fagron	Isosorbide dinitrate 40%	17C29B01350469	1
Fagron	Isosorbide dinitrate 40%	17C29-B01-350469	19
Fagron	Isosorbide dinitrate 40%	17C29-B01-350470	2
Fagron	Isosorbide dinitrate 40%	17C29-B01-352558	4
Fagron	Isosorbide dinitrate 40%	17C29-B01-353161	4
Fagron	Isosorbide dinitrate 40%	17c29-B01-48859	1
Fagron	Isosorbide dinitrate 40%	17C29-Bo1347589	1
Fagron	Isosorbide dinitrate 40%	17c9-b01-347589	1
Fagron	Isosorbide dinitrate 40%	17C-B01-347589	1
Fagron	Isosorbide dinitrate 40%	17V29-B01-347589	1
Fagron	Isosorbide dinitrate 40%	18/18-B01-358241	1
Fagron	Isosorbide dinitrate 40%	18/18-B01-359177	2
Fagron	Isosorbide dinitrate 40%	18/18-B01-359178	2
Fagron	Isosorbide dinitrate 40%	18-18-b01-358242	2
Fagron	Isosorbide dinitrate 40%	1818b01359178	5
Fagron	Isosorbide dinitrate 40%	1818B01373439	1
Fagron	Isosorbide dinitrate 40%	1818bo1373439	1
Fagron	Isosorbide dinitrate 40%	18J118-B01-363844	1
Fagron	Isosorbide dinitrate 40%	18J18_B01_358247	1
Fagron	Isosorbide dinitrate 40%	18J18_B01_373439	1
Fagron	Isosorbide dinitrate 40%	18J18-01-370272	1
Fagron	Isosorbide dinitrate 40%	18J18-01-373438	1
Fagron	Isosorbide dinitrate 40%	18j18-B01	1
Fagron	Isosorbide dinitrate 40%	18J18-B01	20
Fagron	Isosorbide dinitrate 40%	18J18-B01-258241	1
Fagron	Isosorbide dinitrate 40%	18J18-B01-263844	1
Fagron	Isosorbide dinitrate 40%	18J18-B01-3395177	1
Fagron	Isosorbide dinitrate 40%	18J18-B01-358241	27
Fagron	Isosorbide dinitrate 40%	18J18B01358242	1
Fagron	Isosorbide dinitrate 40%	18J18-B01-358242	1
Fagron	Isosorbide dinitrate 40%	18J18-B01-358247	16
Fagron	Isosorbide dinitrate 40%	18j18-b01-359177	1
Fagron	Isosorbide dinitrate 40%	18J18-B01359177	2
Fagron	Isosorbide dinitrate 40%	18J18-B01-359177	38
Fagron	Isosorbide dinitrate 40%	18J-18-B01-359177	1
Fagron	Isosorbide dinitrate 40%	18J18B01359178	1
Fagron	Isosorbide dinitrate 40%	18J18-B01-359178	10

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Isosorbide dinitrate 40%	18J18-B01359579	1
Fagron	Isosorbide dinitrate 40%	18J18B01361397	1
Fagron	Isosorbide dinitrate 40%	18J18-B01-3638345	1
Fagron	Isosorbide dinitrate 40%	18J18-b01-363844	1
Fagron	Isosorbide dinitrate 40%	18J18-B01-363844	24
Fagron	Isosorbide dinitrate 40%	18j18-b01-363845	1
Fagron	Isosorbide dinitrate 40%	18J18B01363845	1
Fagron	Isosorbide dinitrate 40%	18J18B01-363845	1
Fagron	Isosorbide dinitrate 40%	18J18-B01-363845	26
Fagron	Isosorbide dinitrate 40%	18j18-b01-363846	1
Fagron	Isosorbide dinitrate 40%	18J18-B01-363846	5
Fagron	Isosorbide dinitrate 40%	18J18B01365264	1
Fagron	Isosorbide dinitrate 40%	18J18-B01-3702702	1
Fagron	Isosorbide dinitrate 40%	18j18-b01-370272	1
Fagron	Isosorbide dinitrate 40%	18J18B01370272	1
Fagron	Isosorbide dinitrate 40%	18J18-B01-370272	38
Fagron	Isosorbide dinitrate 40%	18J18b01373438	1
Fagron	Isosorbide dinitrate 40%	18J18B01-373438	1
Fagron	Isosorbide dinitrate 40%	18J18-B01-373438	12
Fagron	Isosorbide dinitrate 40%	18J18-B01-373439	2
Fagron	Isosorbide dinitrate 40%	18J18-BO1-359177	1
Fagron	Isosorbide dinitrate 40%	18J18-BO1-3702702	1
Fagron	Isosorbide dinitrate 40%	18J18-BO1-373438	2
Fagron	Isosorbide dinitrate 40%	18J19-B01	1
Fagron	Isosorbide dinitrate 40%	1934469	1
Fagron	Isosorbide dinitrate 40%	193469	12
Fagron	Isosorbide dinitrate 40%	195293	26
Fagron	Isosorbide dinitrate 40%	2114M3516	1
Fagron	Isosorbide dinitrate 40%	2203089	6
Fagron	Isosorbide dinitrate 40%	22D11-B05-215487	11
Fagron	Isosorbide dinitrate 40%	22D11-B05-215525	8
Fagron	Isosorbide dinitrate 40%	22D11-B05-216314	13
Fagron	Isosorbide dinitrate 40%	22D11-B05-216315	1
Fagron	Isosorbide dinitrate 40%	22D11-B05-225756	1
Fagron	Isosorbide dinitrate 40%	22D11-B05-225757	2
Fagron	Isosorbide dinitrate 40%	22D11-BO5	1
Fagron	Isosorbide dinitrate 40%	2413Q03516	1
Fagron	Isosorbide dinitrate 40%	25021711	1
Fagron	Isosorbide dinitrate 40%	2817E-03516	1
Fagron	Isosorbide dinitrate 40%	3115M-03516	1
Fagron	Isosorbide dinitrate 40%	3211U-03516	1
Fagron	Isosorbide dinitrate 40%	3413U03516	1
Fagron	Isosorbide dinitrate 40%	3518M-03516	1
Fagron	Isosorbide dinitrate 40%	359177	2
Fagron	Isosorbide dinitrate 40%	391311-03516	1
Fagron	Isosorbide dinitrate 40%	4314U-03516	1
Fagron	Isosorbide dinitrate 40%	517I-03516	1
Fagron	Isosorbide dinitrate 40%	701319-0001	1
Fagron	Isosorbide dinitrate 40%	7013190003	1
Fagron	Isosorbide dinitrate 40%	8564340	1
Fagron	Isosorbide dinitrate 40%	9101205	1
Fagron	Isosorbide dinitrate 40%	9E05-N05	1
Fagron	Isosorbide dinitrate 40%	B01-3591707	2
Fagron	Isosorbide dinitrate 40%	B01-3591708	1
Fagron	Isosorbide dinitrate 40%	B01-3638404	8
Fagron	Isosorbide dinitrate 40%	B01-3638406	2
Fagron	Isosorbide dinitrate 40%	B01-363844	1
Fagron	Isosorbide dinitrate 40%	B01-3702702	10
Fagron	Isosorbide dinitrate 40%	B01-3734308	2
Fagron	Isosorbide dinitrate 40%	B013734309	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Isosorbide dinitrate 40%	B01-3734309	1
Fagron	Isosorbide dinitrate 40%	B05-2154807	1
Fagron	Isosorbide dinitrate 40%	B05-2163104	1
Fagron	Isosorbide dinitrate 40%	IN20012021	1
Fagron	Isosorbide dinitrate 40%	P11008	1
Fagron	Isosorbide dinitrate 40%	testxx	1
Fagron	Isosorbide dinitrate 40%	X12010	1
Fargon / AHD	Isosorbide dinitrate 40%	18J18-B01-363844	1
Fargon/Gehe	Isosorbide dinitrate 40%	15/10-B01-331286	1
Fargon/Gehe	Isosorbide dinitrate 40%	17C29-B01-339447	1
Fargon/Gehe	Isosorbide dinitrate 40%	17C29-B01-348859	1
Fargon/Gehe	Isosorbide dinitrate 40%	18J18-B01-373438	1
Fargon/Noweda	Isosorbide dinitrate 40%	18j18-B01-359177	1
Fargon/Spangro	Isosorbide dinitrate 40%	195293	1
Fargon	Isosorbide dinitrate 40%	15/10-B01-320081	1
Fargon	Isosorbide dinitrate 40%	17C29-B01	1
Fargon	Isosorbide dinitrate 40%	18J18-B01	3
Fargon	Isosorbide dinitrate 40%	18J18-B01-363845	1
Fargron / Gehe	Isosorbide dinitrate 40%	17C29-B01-339447	1
Fiebig 23.05.13 ek: ...	Isosorbide dinitrate 40%	12F08-N04	1
Fiebig	Isosorbide dinitrate 40%	17C29-B01-350469	1
Fiebig	Isosorbide dinitrate 40%	18j18-b01-358247	1
Fiebig	Isosorbide dinitrate 40%	18J18-B01-359177	1
Fiebig	Isosorbide dinitrate 40%	18J18-B01-363844	1
Fiebig	Isosorbide dinitrate 40%	18J18-B01-363846	1
Fiebig	Isosorbide dinitrate 40%	bo1-3702702	1
Frago/Gehe	Isosorbide dinitrate 40%	17C29-B01-335070	1
Frago/Noweda	Isosorbide dinitrate 40%	15I10-B01-328577	1
Gehe amax	Isosorbide dinitrate 40%	15I10-B01-331286	1
Gehe amax	Isosorbide dinitrate 40%	18J18-B01-363844	1
Gehe amax	Isosorbide dinitrate 40%	18J18-B01-363845	2
Gehe amax	Isosorbide dinitrate 40%	18J18-B01-370272	1
Gehe	Isosorbide dinitrate 40%	17c29-B01-335070	1
GEHE	Isosorbide dinitrate 40%	17C29-B01-347589	1
Gehe	Isosorbide dinitrate 40%	18J18-B01	1
Gehe	Isosorbide dinitrate 40%	18J18-B01-358241	1
Gehe	Isosorbide dinitrate 40%	18J18-B01-358247	1
Gehe	Isosorbide dinitrate 40%	18J18-B01-373438	1
Gehe	Isosorbide dinitrate 40%	22D11-B05-216314	1
Gehe	Isosorbide dinitrate 40%	22D11-B05-225756	1
Gehe	Isosorbide dinitrate 40%	B01-3702702	1
Ichthyol-Gesellschaft	Isosorbide dinitrate 40%	17C29-B01-335070	1
Kehr	Isosorbide dinitrate 40%	200051401	1
Kehr	Isosorbide dinitrate 40%	22D11-B05-216314	1
Krieger	Isosorbide dinitrate 40%	3186	1
L12	Isosorbide dinitrate 40%	149168	1
L12	Isosorbide dinitrate 40%	15I10-B01-331286	2
Noweda / Fargon	Isosorbide dinitrate 40%	18j18-B01	1
Noweda	Isosorbide dinitrate 40%	15/10-B01-315217	1
Noweda	Isosorbide dinitrate 40%	15I10-B01-331287	1
Noweda	Isosorbide dinitrate 40%	17C29-B01-350469	1
Noweda	Isosorbide dinitrate 40%	17C29-B01-352558	1
Noweda	Isosorbide dinitrate 40%	195293	1
Noweda	Isosorbide dinitrate 40%	22D11-B05-225756	2
Phoenix	Isosorbide dinitrate 40%	3066	1
Phoenix	Isosorbide dinitrate 40%	3362	1
Phönix	Isosorbide dinitrate 40%	13A07-N13	1
Sanacorp	Isosorbide dinitrate 40%	11J17-N05	1
Sanacorp	Isosorbide dinitrate 40%	14D09-B03-294280	1
Sanacorp	Isosorbide dinitrate 40%	18J18-B01-358241	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Isosorbide dinitrate 40%	18J18-B01-358247	2
Sanacorp	Isosorbide dinitrate 40%	18J18-B01-359177	1
Sanacorp	Isosorbide dinitrate 40%	18J18-B01-363845	1
Sanacorp	Isosorbide dinitrate 40%	18J18-B01-363846	1
Sanacorp	Isosorbide dinitrate 40%	193469	1
Sanacorp	Isosorbide dinitrate 40%	22d11-b05-215525	1
Sanacorp	Isosorbide dinitrate 40%	22D11-B05-216314	1
Sanacorp	Isosorbide dinitrate 40%	22D11-B05-229443	2
UCB manufacturing Ireland	Isosorbide dinitrate 40%	14D09-B03-300234	2
VDl 28.10.14 10,32 euro	Isosorbide dinitrate 40%		1
VDL	Isosorbide dinitrate 40%	18J18-B01-358247	1
Wepa	Isosorbide dinitrate 40%	14D09-B03-313566	1

- 235 013 spectra from 1515 *Apo-Ident* customers from a total of 48 990 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Isosorbide dinitrate 40%* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Isosorbide dinitrate 40%* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	229	0	152 733
Type B	0	150	0	201 934
Type C	0	1040	14	235 013

The substance/substance group *Isosorbide dinitrate 40%* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.3799 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9007 %)	98.6717 % (> 98.3871 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20891	23200	14.42	189.73
21347	23200	7.55	190.76
23200	23200	0.00	184.45
23598	23200	8.21	185.41
24057	23200	10.35	182.71
27044	23200	8.23	177.66

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Isoxsuprine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	22640-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Isoxsuprine hydrochloride; Isoxsuprini hydrochloridum

Special notes

When selecting the *Isoxsuprine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Isoxsuprine hydrochloride	7	3	0

Second-stage model

For differentiation of the substance/substance group *Isoxsuprine hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Isoxsuprine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	107.31	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Isoxsuprine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Isoxsuprine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Isoxsuprine hydrochloride	161770	22640	40	20160818*
Caelo	Isoxsuprine hydrochloride	16177001	22735	40	20160818
Caelo	Isoxsuprine hydrochloride	181078	24252	40	20180719*
Euro OTC	Isoxsuprine hydrochloride	1503008-01	22659	40	20150430
Euro OTC	Isoxsuprine hydrochloride	1905019	24920	40	20191128*
Euro OTC	Isoxsuprine hydrochloride	2006035	25285	40	20200706*
Fagron	Isoxsuprine hydrochloride	22I21-B01-233784	27051	40	20230714
Fagron	Isoxsuprine hydrochloride	22I21-B01-233784	27051SI	20	20230714

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 300 spectra of 8 reference samples from the substance/substance group *Isoxsuprine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 662 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Isoxsuprine hydrochloride*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Isoxsuprine hydrochloride	190117	24547	40
Euro OTC	Isoxsuprine hydrochloride	2106006	25760	50
Fagron	Isoxsuprine hydrochloride	20L09-B12-213682	26322	30
Fagron	Isoxsuprine hydrochloride	20L09-B12-213682	26322SI	20

- 201 944 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Isoxsuprine hydrochloride*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Isoxsuprine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Isoxsuprine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	140	0	201 944
Type C	0	0	0	236 067

The substance/substance group *Isoxsuprine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22640	22640	0.00	198.55
22659	22640	5.22	199.87
22735	22640	4.92	196.12
24252	24252	0.00	201.23
24920	24920	0.00	191.60
25285	25285	0.00	195.27
27051	22640	7.56	197.95

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ivermectin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10006049-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ivermectin; Ivermectinum

Special notes

When selecting the *Ivermectin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ivermectin	2	1	0

Second-stage model

For differentiation of the substance/substance group *Ivermectin* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ivermectin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	95.49	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ivermectin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ivermectin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ivermectin	23L22-H07-00747	27067	40	20231228
Fagron	Ivermectin	23L22-H07-00747	27067SI	20	20231228
FSA Chemicals	Ivermectin	23J18-AP24014	27217	40	241107538

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 100 spectra of 3 reference samples from the substance/substance group *Ivermectin*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 862 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 3 reference samples from the substance/substance group *Ivermectin*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ivermectin	22E06-H05-00747	26404	40
Fagron	Ivermectin	22E06-H05-00747	26404SI	20
FSA Chemicals	Ivermectin	23J18-AP24014	27217SI†	20

- 202 004 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Ivermectin*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ivermectin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ivermectin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

	False positive	True positive	False negative	True negative
Type A	0	100	0	152 862
Type B	0	80	0	202 004
Type C	0	0	0	236 067

The substance/substance group *Ivermectin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
27067	27217	73.61	137.57
27217	27217	0.00	136.92

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ketamine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20278-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ketamine hydrochloride; Ketamini hydrochloridum

Special notes

When selecting the *Ketamine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ketamine hydrochloride	6	5	88

Second-stage model

For differentiation of the substance/substance group *Ketamine hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ketamine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Omeprazole	115.04	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ketamine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ketamine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Ketamine hydrochloride	2304005	26658	40	20230419*
Fagron	Ketamine hydrochloride	13H19-N01	21044	40	8931
Fagron	Ketamine hydrochloride	14I03-B02-303165	21779	60	20140926
Fagron	Ketamine hydrochloride	14I03-B02-311706	22533	40	20140926
Fagron	Ketamine hydrochloride	19H14-F02-364305	25295	40	20190918
Fagron	Ketamine hydrochloride	22F01-F01-385041	26909	40	20230727

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 260 spectra of 6 reference samples from the substance/substance group *Ketamine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 270 spectra of 8 reference samples from the substance/substance group *Ketamine hydrochloride*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ketamine hydrochloride	15E07-B03-322164	23201	40
Fagron	Ketamine hydrochloride	16E18-B03-339897	23941	40
Fagron	Ketamine hydrochloride	21D30-F02-378537	25759	40
Gatt-Koller	Ketamine hydrochloride	23J00824	26989	40
Gatt-Koller	Ketamine hydrochloride	23J01507	26990	40
Euro OTC	Ketamine hydrochloride	2304005	26658SI†	20
Fagron	Ketamine hydrochloride	21D30-F02-378537	25759SI	10
Fagron	Ketamine hydrochloride	22F01-F01-385041	26909SI†	40

- 201 814 spectra from a total of 4038 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 261 spectra from 110 *Apo-Ident* customers from 97 batches from the substance/substance group *Ketamine hydrochloride*.

- Among them are spectra of independent samples from 88 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Ketamine hydrochloride	22F01-385047	1
	Ketamine hydrochloride	22F01-F01-385041	2
	Ketamine hydrochloride	2304005-01	5
	Ketamine hydrochloride	2304005-02	1
	Ketamine hydrochloride	2304005-03	5
	Ketamine hydrochloride	2304005-04	1
	Ketamine hydrochloride	2IL-13-F02-383873	1
AHD	Ketamine hydrochloride	2304005-02	1
Allergika Pharma / Phönix	Ketamine hydrochloride	21L13-F02-383872	1
Alliance Healthcare	Ketamine hydrochloride	21L13-F02-383872	1
Caelo	Ketamine hydrochloride	17K14-B01-355067	1
Caelo	Ketamine hydrochloride	21D30-F02-378863	1
Caesar & Loretz GmbH	Ketamine hydrochloride	700932-0001	1
Euro OTC	Ketamine hydrochloride	21D30-F02-378537	2
Euro OTC	Ketamine hydrochloride	21D3O-F02-378537	1
Euro OTC	Ketamine hydrochloride	2304005-01	1
Euro OTC	Ketamine hydrochloride	2304005-02	1
Euro OTC	Ketamine hydrochloride	F04-3734305	1
Fagron	Ketamine hydrochloride	/0321025	1
Fagron	Ketamine hydrochloride	14/03-B02-303165	1
Fagron	Ketamine hydrochloride	14/03-B02-309852	1
Fagron	Ketamine hydrochloride	14I03-B02-303165	1
Fagron	Ketamine hydrochloride	14I03-B02-309852	1
Fagron	Ketamine hydrochloride	15E07-B03-322164	5
Fagron	Ketamine hydrochloride	15E07-B03-327604	3
Fagron	Ketamine hydrochloride	16E18-B03	1
Fagron	Ketamine hydrochloride	16E18-B03-328264	2
Fagron	Ketamine hydrochloride	16E18-B03-330627	1
Fagron	Ketamine hydrochloride	16E18-B03-332957	3
Fagron	Ketamine hydrochloride	16E18-B03-334369	3
Fagron	Ketamine hydrochloride	16E18-B03-334370	1
Fagron	Ketamine hydrochloride	16E18-B03-335529	1
Fagron	Ketamine hydrochloride	16E18-B03-339897	4
Fagron	Ketamine hydrochloride	16E18-B03-339898	1
Fagron	Ketamine hydrochloride	16E18-B03-345971	2
Fagron	Ketamine hydrochloride	173017P	3
Fagron	Ketamine hydrochloride	17K14-B01-347995	4
Fagron	Ketamine hydrochloride	17K14-B01-347996	4
Fagron	Ketamine hydrochloride	17K14-B01-347997	1
Fagron	Ketamine hydrochloride	17K14-B01-3533344	1
Fagron	Ketamine hydrochloride	17K14B01353344	1
Fagron	Ketamine hydrochloride	17K14-B01-353344	1
Fagron	Ketamine hydrochloride	17K14-B01-356831	6
Fagron	Ketamine hydrochloride	17K14-B01-358396	8
Fagron	Ketamine hydrochloride	17K14-B01-358397	2
Fagron	Ketamine hydrochloride	182513P	1
Fagron	Ketamine hydrochloride	19H14-F02	6
Fagron	Ketamine hydrochloride	19h14-f02-364305	1
Fagron	Ketamine hydrochloride	19H14-F02-364305	9
Fagron	Ketamine hydrochloride	19H14-F02-364306	2
Fagron	Ketamine hydrochloride	19H14-F02-3650504	1
Fagron	Ketamine hydrochloride	19H14-F02365054	1
Fagron	Ketamine hydrochloride	19H14-F02-365054	5
Fagron	Ketamine hydrochloride	19H14-F07-3643005	1
Fagron	Ketamine hydrochloride	20A07-F01	2
Fagron	Ketamine hydrochloride	20a07-f01-368076	1
Fagron	Ketamine hydrochloride	20A07-F01368076	1
Fagron	Ketamine hydrochloride	20A07-F01-368076	8
Fagron	Ketamine hydrochloride	20A07-F01-368077	5
Fagron	Ketamine hydrochloride	20A07-F01-368078	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Ketamine hydrochloride	20A07-F01-3697602	1
Fagron	Ketamine hydrochloride	20A07-F01-369762	3
Fagron	Ketamine hydrochloride	20A07-F01-369763	3
Fagron	Ketamine hydrochloride	20G12-F04-373435	1
Fagron	Ketamine hydrochloride	20G13-F04	8
Fagron	Ketamine hydrochloride	20G13-F04-3729706	1
Fagron	Ketamine hydrochloride	20G13-F04-3729707	1
Fagron	Ketamine hydrochloride	20G13-F04-372976	1
Fagron	Ketamine hydrochloride	20G13-F04-372979	1
Fagron	Ketamine hydrochloride	20G13-F04-372981	1
Fagron	Ketamine hydrochloride	20G13-F04-373435	4
Fagron	Ketamine hydrochloride	21D033-F02-378538	1
Fagron	Ketamine hydrochloride	21D03-F02-378537	1
Fagron	Ketamine hydrochloride	21D30-F02	6
Fagron	Ketamine hydrochloride	21D30-F02-378537	6
Fagron	Ketamine hydrochloride	21D30-F02-378538	4
Fagron	Ketamine hydrochloride	21d30-F02-378863	1
Fagron	Ketamine hydrochloride	21D30-F02-378863	9
Fagron	Ketamine hydrochloride	21D30Fo2378537	1
Fagron	Ketamine hydrochloride	21D3OF02378537	1
Fagron	Ketamine hydrochloride	21L13-F02	1
Fagron	Ketamine hydrochloride	21L13-F02-380925	13
Fagron	Ketamine hydrochloride	21L13-F02-381974	10
Fagron	Ketamine hydrochloride	21L13-F02-383872	4
Fagron	Ketamine hydrochloride	21L13-F02-383873	2
Fagron	Ketamine hydrochloride	21L13-F02-381974	2
Fagron	Ketamine hydrochloride	F0136807006	1
Fagron	Ketamine hydrochloride	F01-3680707	1
Fagron	Ketamine hydrochloride	F02-3650504	1
Fagron	Ketamine hydrochloride	f02-3785307	1
Fagron	Ketamine hydrochloride	F02-3785307	1
Fagron	Ketamine hydrochloride	F02-3785308	1
Fagron	Ketamine hydrochloride	F04-3734305	3
Fagron	Ketamine hydrochloride	F02-3788603	1
Fagron	Ketamine hydrochloride	SLL/KH/0321025	1
Fagron	Ketamine hydrochloride	SLL/KH/0422074	2
Fagron	Ketamine hydrochloride	SLL/KH/0520042	3
Fagron	Ketamine hydrochloride	SLL/KH/0719030	1
Fargon/Noweda	Ketamine hydrochloride	17K14-B01-356831	1
Fargron / Gehe	Ketamine hydrochloride	20G13-F04-373435	1
Gatt-Koller	Ketamine hydrochloride	1803056	1
GEHE 27.05.2014	Ketamine hydrochloride	13H19-N01	1
Gehe	Ketamine hydrochloride	19H14-F02-364305	1
Gehe	Ketamine hydrochloride	20A07-F01-368077	1
Gehe	Ketamine hydrochloride	20G13-F04-372976	1
Gehe	Ketamine hydrochloride	21D30-F02-378538	1
Gehe	Ketamine hydrochloride	22F01-F01-385041	2
jenne	Ketamine hydrochloride	2304005	1
Noweda	Ketamine hydrochloride	14/03-B02-311706	1
Noweda	Ketamine hydrochloride	292414P	1
Phoenix	Ketamine hydrochloride	F01-3680708	2
phönix	Ketamine hydrochloride	14103-B02-311706	1
Sanacorp	Ketamine hydrochloride	22F01-F01-385041	1

- 235 806 spectra from 1515 *Apo-Ident* customers from a total of 49 161 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ketamine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ketamine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	270	0	201 814
Type C	0	258	3	235 806

The substance/substance group *Ketamine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.7778 %)
Type C	100.0000 % (> 99.9007 %)	98.8506 % (> 97.7011 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21044	21044	0.00	133.89
21779	21044	15.04	138.29
22533	21044	8.56	133.35
25295	26658	10.73	131.93
26658	26658	0.00	128.86
26909	21044	57.51	114.20

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ketoconazole**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20688-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ketoconazole; Ketoconazolum

Special notes

When selecting the *Ketoconazole* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ketoconazole	6	3	77

Second-stage model

For differentiation of the substance/substance group *Ketoconazole* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ketoconazole* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Midazolam hydrochloride	116.96	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ketoconazole* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ketoconazole*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ketoconazole	12171007	20688	30	1401554
Caelo	Ketoconazole	13179612	21514	60	20130613
Caelo	Ketoconazole	13179612	21515	60	20130613
Caelo	Ketoconazole	153477	24028	40	20151113*
Fagron	Ketoconazole	12A16-N06	20699	40	20120123
Fagron	Ketoconazole	16A26-B01-322982	23183	40	20160210
Fagron	Ketoconazole	20H18-F03-375993	25666	50	20201116

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 320 spectra of 7 reference samples from the substance/substance group *Ketoconazole*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 5 reference samples from the substance/substance group *Ketoconazole*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ketoconazole	20002966003	25430	40
Fagron	Ketoconazole	17H14-B01-339422	23917	40
Fagron	Ketoconazole	21K18-B06-213329	26281	40
Fagron	Ketoconazole	20H18-F03-375993	25666SI†	10
Fagron	Ketoconazole	21K18-B06-213329	26281SI	20

- 201 934 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 258 spectra from 145 *Apo-Ident* customers from 80 batches from the substance/substance group *Ketoconazole*.

- Among them are spectra of independent samples from 77 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Ketoconazole	20003758006	1
	Ketoconazole	20003758009	2
	Ketoconazole	20003758017	1
	Ketoconazole	21k18-b06	1
Alliance Healthcare	Ketoconazole	20002966003	1
ANZAG 23.07.14	Ketoconazole	13h09-n07	1
Caelo	Ketoconazole	11070001	1
Caelo	Ketoconazole	11070022	1
Caelo	Ketoconazole	12300406	1
Caelo	Ketoconazole	12300407	2
Caelo	Ketoconazole	13179601	2
Caelo	Ketoconazole	13179606	3
Caelo	Ketoconazole	13179612	2
Caelo	Ketoconazole	13399404	8
Caelo	Ketoconazole	13399408	7
Caelo	Ketoconazole	13399412	3
Caelo	Ketoconazole	14350408	4
Caelo	Ketoconazole	14350416	4
Caelo	Ketoconazole	14350419	1
Caelo	Ketoconazole	14350420	2
Caelo	Ketoconazole	14350421	1
Caelo	Ketoconazole	14350422	3
Caelo	Ketoconazole	14350427	2
Caelo	Ketoconazole	14350429	6
Caelo	Ketoconazole	14350434	2
Caelo	Ketoconazole	14350436	3
Caelo	Ketoconazole	14350437	7
Caelo	Ketoconazole	14350442	3
Caelo	Ketoconazole	14k04-b06-309671	1
Caelo	Ketoconazole	15347701	13
Caelo	Ketoconazole	18007003	6
Caelo	Ketoconazole	18007004	2
Caelo	Ketoconazole	18007011	5
Caelo	Ketoconazole	18007013	2
Caelo	Ketoconazole	18007015	9
Caelo	Ketoconazole	18007016	1
Caelo	Ketoconazole	18007020	2
Caelo	Ketoconazole	1906611	1
Caelo	Ketoconazole	19096601	6
Caelo	Ketoconazole	19096605	2
Caelo	Ketoconazole	19096609	1
Caelo	Ketoconazole	19096611	4
Caelo	Ketoconazole	20002966001	1
Caelo	Ketoconazole	20002966002	2
Caelo	Ketoconazole	20002966003	9
Caelo	Ketoconazole	20003758004	4
Caelo	Ketoconazole	20003758005	6
Caelo	Ketoconazole	20003758006	2
Caelo	Ketoconazole	20003758009	1
Caelo	Ketoconazole	2003758005	1
Caelo	Ketoconazole	53317046	2
Caeolo /Gehe	Ketoconazole	14350408	1
Caesar & Loretz GmbH...	Ketoconazole	19096601	1
Caesar & Loretz GmbH/AHD	Ketoconazole	19096611	1
Caesar & Loretz GmbH/AHD	Ketoconazole	20003758005	1
Caesar & Loretz GmbH...	Ketoconazole	19096601	1
Caesar & Loretz GmbH...	Ketoconazole	19096611	1
Caesar & Loretz GmbH/Gehe	Ketoconazole	20003758005	1
Caesar & Loretz GmbH...	Ketoconazole	20002966003	2
Caesar & Loretz GmbH...	Ketoconazole	20002966003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Ketoconazole	20003758004	2
Caesar & Loretz GmbH	Ketoconazole	18007015	2
Caesar & Loretz GmbH	Ketoconazole	19096601	1
Caesar & Loretz GmbH	Ketoconazole	19096608	1
Caesar & Loretz GmbH	Ketoconazole	19096611	2
Caesar & Loretz GmbH	Ketoconazole	20002966002	1
Caesar & Loretz GmbH	Ketoconazole	20002966003	9
Caesar & Loretz GmbH	Ketoconazole	20003758004	4
Caesar & Loretz GmbH	Ketoconazole	20003758005	4
Caesar & Loretz GmbH	Ketoconazole	20003758006	3
Caesar & Loretz/AHD	Ketoconazole	18007015	1
E Plus	Ketoconazole	14350429	1
Euro OTC	Ketoconazole	13179615	1
Fagron	Ketoconazole	12I17-N02	1
Fagron	Ketoconazole	13179613	1
Fagron	Ketoconazole	13H09-N07	1
Fagron	Ketoconazole	13J23-N04	1
Fagron	Ketoconazole	14E09-B01-293736	3
Fagron	Ketoconazole	14E09-B01-297637	2
Fagron	Ketoconazole	14K04-B06-309671	3
Fagron	Ketoconazole	15G23-B03-312063	1
Fagron	Ketoconazole	15G23-B03-316596	2
Fagron	Ketoconazole	16A26-B01-327490	1
Fagron	Ketoconazole	16A26-B01-335467	3
Fagron	Ketoconazole	17H14-B01-339006	1
Fagron	Ketoconazole	17H14-B01-339422	1
Fagron	Ketoconazole	17H14-B01-344222	2
Fagron	Ketoconazole	17H14-B01-353376	1
Fagron	Ketoconazole	17h14-b01-353378	1
Fagron	Ketoconazole	17H14-B01-353378	1
Fagron	Ketoconazole	18E28-B02-359205	2
Fagron	Ketoconazole	18E28-B02-364169	4
Fagron	Ketoconazole	20h18-F03-375071	1
Fagron	Ketoconazole	20H18-F03-375071	2
Fagron	Ketoconazole	20H18-F03-375073	1
Fagron	Ketoconazole	21k18-bo6	1
Fagron	Ketoconazole	5015E-02866	1
Fagron	Ketoconazole	700669-0001	1
Fagron	Ketoconazole	KET/11707237	1
Fagron	Ketoconazole	KET/12007311	1
Fiebig	Ketoconazole	14350437	1
Fiebig	Ketoconazole	19096601	1
Gehe	Ketoconazole	11070019	1
Gehe	Ketoconazole	14350427	1
Gehe	Ketoconazole	20003758009	1
Noweda	Ketoconazole	19096601	1
Phoenix	Ketoconazole	19096601	1
Phönix/Caesar&Lorenz...	Ketoconazole	20003758005	1
Phönix	Ketoconazole	12171018	1
Phönix	Ketoconazole	13179602	3
Phönix	Ketoconazole	18007003	1
Sanacorp Stralsund	Ketoconazole	20003758005	1
Sanacorp	Ketoconazole	20003758006	3

- 235 809 spectra from 1515 *Apo-Ident* customers from a total of 49 178 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ketoconazole* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ketoconazole* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	150	0	201 934
Type C	0	255	3	235 809

The substance/substance group *Ketoconazole* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9007 %)	98.8372 % (> 97.6744 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20688	20688	0.00	205.65
20699	24028	12.27	210.53
21514	24028	10.45	210.41
21515	24028	19.37	206.13
23183	24028	18.30	210.36
24028	24028	0.00	212.29
25666	24028	30.64	202.29

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Lactose monohydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20029-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lactose monohydrate; Lactosum monohydricum

Special notes

When selecting the *Lactose monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Lactose monohydrate	6	14	521

Second-stage model

For differentiation of the substance/substance group *Lactose monohydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Lactose monohydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Pancreas powder	35.41	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Lactose monohydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Lactose monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Lactose monohydrate	12139910	20685	30	20120606
Caelo	Lactose monohydrate	14025601	21525	40	20140207
Caelo	Lactose monohydrate	14025601	21526	40	20140207
Caelo	Lactose monohydrate	14025601	21527	40	20140207
Caelo	Lactose monohydrate	14025601	21528	40	20140207
Caelo	Lactose monohydrate	14025601	21529	40	20140207
Caelo	Lactose monohydrate	160277	22460	60	20160321*
Euro OTC	Lactose monohydrate	1509030	21935	60	20151013*
Euro OTC	Lactose monohydrate	1606025	22701	40	20160628*
Euro OTC	Lactose monohydrate	1909014	24929	40	20191015*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 430 spectra of 10 reference samples from the substance/substance group *Lactose monohydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 532 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 620 spectra of 17 reference samples from the substance/substance group *Lactose monohydrate*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Lactose monohydrate	15236220	22584	40
Caelo	Lactose monohydrate	173360	23828	40
Caelo	Lactose monohydrate	192364	25233	40
Caelo	Lactose monohydrate	191376	25234	40
Caelo	Lactose monohydrate	21001507	25804	50
Caelo	Lactose monohydrate	23001015	26694	40
Caelo	Lactose monohydrate	24001886	27332	40
Euro OTC	Lactose monohydrate	1703019	23141	40
Euro OTC	Lactose monohydrate	1802002	23962	40
Euro OTC	Lactose monohydrate	1812008	24415	40
Euro OTC	Lactose monohydrate	2005026	25275	40
Euro OTC	Lactose monohydrate	2201013	25952	40
Euro OTC	Lactose monohydrate	2208008	26277	40
Euro OTC	Lactose monohydrate	2309012	27012	40
Caelo	Lactose monohydrate	23001015	26694SI	20
Euro OTC	Lactose monohydrate	2201013	25952SI	10
Euro OTC	Lactose monohydrate	2208008	26277SI	20

- 201 464 spectra from a total of 4031 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2465 spectra from 667 *Apo-Ident* customers from 526 batches from the substance/substance group *Lactose monohydrate*.

- Among them are spectra of independent samples from 521 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Lactose monohydrate	14025604	1
	Lactose monohydrate	2005026-02	1
	Lactose monohydrate	22000736005	1
	Lactose monohydrate	22000736007	1
	Lactose monohydrate	22000736008	3
	Lactose monohydrate	22000736010	1
	Lactose monohydrate	22000736012	1
	Lactose monohydrate	22000736016	2
	Lactose monohydrate	22000736018	3
	Lactose monohydrate	2208008-01	1
	Lactose monohydrate	2208008-02	1
	Lactose monohydrate	2208008-03	3
	Lactose monohydrate	23001015001	4
	Lactose monohydrate	23001015003	13
	Lactose monohydrate	23001015004	11
	Lactose monohydrate	23001015007	3
	Lactose monohydrate	23002236002	11
	Lactose monohydrate	23002236003	8
	Lactose monohydrate	23002236005	2
	Lactose monohydrate	23003217001	4
	Lactose monohydrate	23003217003	4
	Lactose monohydrate	23003217009	1
	Lactose monohydrate	2309012-01	2
	Lactose monohydrate	309351/0	1
	Lactose monohydrate	309508/0	1
A.H.D.	Lactose monohydrate	12336801	1
AEP	Lactose monohydrate	18198007	2
AHD	Lactose monohydrate	13I23-B03-291114	1
AHD	Lactose monohydrate	15236220	1
AHD	Lactose monohydrate	192364002	1
AHD	Lactose monohydrate	22000736017	1
AHD	Lactose monohydrate	23001015001	1
AHD	Lactose monohydrate	23003217005	1
Alliance H.	Lactose monohydrate	C12H22011	1
Alliance Healthcare	Lactose monohydrate	10195101	2
Alliance Healthcare	Lactose monohydrate	22000736005	1
Alliance	Lactose monohydrate	20004200007	1
Alliance	Lactose monohydrate	22000736018	4
Alliance	Lactose monohydrate	23001015003	1
Alliance	Lactose monohydrate	23003217004	1
Alliance	Lactose monohydrate	23003217009	1
Alte Apotheke	Lactose monohydrate	16027708	1
Anzag / Noweda	Lactose monohydrate	12336815	1
Anzag 29.11.12 ek:7,51	Lactose monohydrate	12139914	1
Anzag/Fragon	Lactose monohydrate	1005SLP	1
Anzag	Lactose monohydrate	12139915	5
Anzag	Lactose monohydrate	192364014	1
api-ident	Lactose monohydrate	17078312	1
Bahnhof-Apotheke	Lactose monohydrate	120614	1
Bahnhof-Apotheke	Lactose monohydrate	120808	1
Bahnhof-Apotheke	Lactose monohydrate	121119	2
Bahnhof-Apotheke	Lactose monohydrate	130115	1
Bahnhof-Apotheke	Lactose monohydrate	130729	1
Bahnhof-Apotheke	Lactose monohydrate	130911	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Bahnhof-Apotheke	Lactose monohydrate	130925	1
Bahnhof-Apotheke	Lactose monohydrate	131023	1
Bahnhof-Apotheke	Lactose monohydrate	131112	1
Bahnhof-Apotheke	Lactose monohydrate	131127	2
Bahnhof-Apotheke	Lactose monohydrate	131218	2
Bahnhof-Apotheke	Lactose monohydrate	140113	3
Bahnhof-Apotheke	Lactose monohydrate	140206	2
Bahnhof-Apotheke	Lactose monohydrate	140220	1
Bahnhof-Apotheke	Lactose monohydrate	140310	2
Bahnhof-Apotheke	Lactose monohydrate	140630	1
Bahnhofsapotheke	Lactose monohydrate	140401	1
Bären Apotheke	Lactose monohydrate	16231206	1
Bombastus	Lactose monohydrate	13299108	1
Bombastus	Lactose monohydrate	17000754	1
Bombastus	Lactose monohydrate	17001199	1
Bombastus	Lactose monohydrate	17001212	1
Bombastus	Lactose monohydrate	17078302	1
Bombastus	Lactose monohydrate	272680/0	1
Bombastus	Lactose monohydrate	274926	1
Bombastus	Lactose monohydrate	275194/0	1
Bombastus	Lactose monohydrate	275225/0	1
Bombastus	Lactose monohydrate	282648	1
Bombastus	Lactose monohydrate	282696/0	1
Bombastus	Lactose monohydrate	283992	2
Bombastus	Lactose monohydrate	284321/0	1
Bombastus	Lactose monohydrate	285087/0	1
Bombastus	Lactose monohydrate	286354	1
Bombastus	Lactose monohydrate	286697/0	1
Bombastus	Lactose monohydrate	286710	1
Bombastus	Lactose monohydrate	288015/0	1
Bombastus	Lactose monohydrate	288927	1
Bombastus	Lactose monohydrate	289238	1
Bombastus	Lactose monohydrate	291464	1
Bombastus	Lactose monohydrate	292982	2
Bombastus	Lactose monohydrate	292983	1
Bombastus	Lactose monohydrate	292995	1
Bombastus	Lactose monohydrate	292996	1
Bombastus	Lactose monohydrate	293074	1
Bombastus	Lactose monohydrate	2932880	1
Bombastus	Lactose monohydrate	293289	1
Bombastus	Lactose monohydrate	293290	1
Bombastus	Lactose monohydrate	293649	1
Bombastus	Lactose monohydrate	293918/0	1
Bombastus	Lactose monohydrate	293970	1
Bombastus	Lactose monohydrate	294154	1
Bombastus	Lactose monohydrate	294184/0	1
Bombastus	Lactose monohydrate	294897/0	1
Bombastus	Lactose monohydrate	295011/0	1
Bombastus	Lactose monohydrate	295476	1
Bombastus	Lactose monohydrate	295714	1
Bombastus	Lactose monohydrate	295715	1
Bombastus	Lactose monohydrate	300657	2
Bombastus	Lactose monohydrate	3020165	1
Bombastus	Lactose monohydrate	303658	2
Bombastus	Lactose monohydrate	304755	1
Bombastus	Lactose monohydrate	305227	2
Bombastus	Lactose monohydrate	305227/0	1
Bombastus	Lactose monohydrate	305336	2
Bombastus	Lactose monohydrate	305336/0	1
Bombastus	Lactose monohydrate	306147	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Lactose monohydrate	306651/0	1
Bombastus	Lactose monohydrate	306652	1
Bombastus	Lactose monohydrate	306850	1
Bombastus	Lactose monohydrate	306964	1
Bombastus	Lactose monohydrate	306989	2
Bombastus	Lactose monohydrate	306990	1
Bombastus	Lactose monohydrate	307444/0	1
Bombastus	Lactose monohydrate	307543	2
Bombastus	Lactose monohydrate	307573/0	1
Bombastus	Lactose monohydrate	307702/0	1
Bombastus	Lactose monohydrate	307741	1
Bombastus	Lactose monohydrate	3077410	1
Bombastus	Lactose monohydrate	307976/0	1
Bombastus	Lactose monohydrate	308117	1
Bombastus	Lactose monohydrate	308117/0	1
Bombastus	Lactose monohydrate	308118/0	1
Bombastus	Lactose monohydrate	308438	1
Bombastus	Lactose monohydrate	309351	1
Bombastus	Lactose monohydrate	309413/0	1
Bombastus	Lactose monohydrate	309508	1
Bombastus	Lactose monohydrate	309509	1
Bombastus	Lactose monohydrate	309509/0	1
Bombastus	Lactose monohydrate	310082/0	1
Bombastus	Lactose monohydrate	310691	1
Bombastus	Lactose monohydrate	310691/0	1
Bombastus	Lactose monohydrate	310905	1
Bombastus	Lactose monohydrate	310905/0	1
Bombastus	Lactose monohydrate	310912/0	1
Bombastus	Lactose monohydrate	311280	1
Bombastus	Lactose monohydrate	311280/0	1
Bombastus	Lactose monohydrate	311362/0	1
C21001507004aelo/Gehe	Lactose monohydrate	21001507004	1
Caelo	Lactose monohydrate		3
Caelo	Lactose monohydrate	10071701	1
Caelo	Lactose monohydrate	10195107	2
Caelo	Lactose monohydrate	1071302	1
Caelo	Lactose monohydrate	1090216	1
Caelo	Lactose monohydrate	11014714	1
Caelo	Lactose monohydrate	11041801	1
Caelo	Lactose monohydrate	1106022-02	1
Caelo	Lactose monohydrate	11079002	2
Caelo	Lactose monohydrate	112192	2
Caelo	Lactose monohydrate	11219207	1
Caelo	Lactose monohydrate	11219208	3
Caelo	Lactose monohydrate	11219216	2
Caelo	Lactose monohydrate	12021502	1
Caelo	Lactose monohydrate	12021508	1
Caelo	Lactose monohydrate	12021518	5
Caelo	Lactose monohydrate	12041401	1
Caelo	Lactose monohydrate	12139901	2
Caelo	Lactose monohydrate	12139908	1
Caelo	Lactose monohydrate	12139909	1
Caelo	Lactose monohydrate	12139910	1
Caelo	Lactose monohydrate	12139912	1
Caelo	Lactose monohydrate	12139914	6
Caelo	Lactose monohydrate	12139915	4
Caelo	Lactose monohydrate	12139920	6
Caelo	Lactose monohydrate	12336801	7
Caelo	Lactose monohydrate	12336814	1
Caelo	Lactose monohydrate	12336815	9

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lactose monohydrate	12336816	3
Caelo	Lactose monohydrate	12336820	2
Caelo	Lactose monohydrate	123446test	1
Caelo	Lactose monohydrate	123456	1
Caelo	Lactose monohydrate	123456test	1
Caelo	Lactose monohydrate	12345test	1
Caelo	Lactose monohydrate	1234test	1
Caelo	Lactose monohydrate	12399107	1
Caelo	Lactose monohydrate	123test	6
Caelo	Lactose monohydrate	123Test	4
Caelo	Lactose monohydrate	1301C005	2
Caelo	Lactose monohydrate	13081302	1
Caelo	Lactose monohydrate	13104901	5
Caelo	Lactose monohydrate	13104902	7
Caelo	Lactose monohydrate	13104908	2
Caelo	Lactose monohydrate	13104909	5
Caelo	Lactose monohydrate	13104909-3422310182	1
Caelo	Lactose monohydrate	13104909-3453311172	1
Caelo	Lactose monohydrate	13104910	2
Caelo	Lactose monohydrate	13104911	2
Caelo	Lactose monohydrate	13104912	1
Caelo	Lactose monohydrate	13299101	9
Caelo	Lactose monohydrate	13299102	12
Caelo	Lactose monohydrate	13299103	1
Caelo	Lactose monohydrate	13299107	5
Caelo	Lactose monohydrate	13299108	5
Caelo	Lactose monohydrate	1401003-01	1
Caelo	Lactose monohydrate	1402504	1
Caelo	Lactose monohydrate	14025601	3
Caelo	Lactose monohydrate	14025603	7
Caelo	Lactose monohydrate	14025604	6
Caelo	Lactose monohydrate	14025608	2
Caelo	Lactose monohydrate	14025615	1
Caelo	Lactose monohydrate	14025616	4
Caelo	Lactose monohydrate	14025619	3
Caelo	Lactose monohydrate	14025620	15
Caelo	Lactose monohydrate	140612	3
Caelo	Lactose monohydrate	14140302	4
Caelo	Lactose monohydrate	14140304	2
Caelo	Lactose monohydrate	14140305	8
Caelo	Lactose monohydrate	14140308	7
Caelo	Lactose monohydrate	14140309	2
Caelo	Lactose monohydrate	14140312	14
Caelo	Lactose monohydrate	14333501	3
Caelo	Lactose monohydrate	14333502	2
Caelo	Lactose monohydrate	14333503	1
Caelo	Lactose monohydrate	14333508	1
Caelo	Lactose monohydrate	14333509	10
Caelo	Lactose monohydrate	14333510	1
Caelo	Lactose monohydrate	14333511	5
Caelo	Lactose monohydrate	143335114	1
Caelo	Lactose monohydrate	14333513	7
Caelo	Lactose monohydrate	14333514	1
Caelo	Lactose monohydrate	14333518	4
Caelo	Lactose monohydrate	14333520	10
Caelo	Lactose monohydrate	14333521	8
Caelo	Lactose monohydrate	14333525	1
Caelo	Lactose monohydrate	14333528	2
Caelo	Lactose monohydrate	1433502	1
Caelo	Lactose monohydrate	1433510	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lactose monohydrate	1433518	2
Caelo	Lactose monohydrate	1433520	1
Caelo	Lactose monohydrate	1433521	1
Caelo	Lactose monohydrate	1501017-01	4
Caelo	Lactose monohydrate	15011701	1
Caelo	Lactose monohydrate	15081701	1
Caelo	Lactose monohydrate	150903002	1
Caelo	Lactose monohydrate	1509030-02	1
Caelo	Lactose monohydrate	1523614	1
Caelo	Lactose monohydrate	152362	2
Caelo	Lactose monohydrate	15236201	28
Caelo	Lactose monohydrate	15236202	1
Caelo	Lactose monohydrate	15236203	4
Caelo	Lactose monohydrate	15236204	11
Caelo	Lactose monohydrate	15236206	1
Caelo	Lactose monohydrate	15236208	13
Caelo	Lactose monohydrate	15236209	12
Caelo	Lactose monohydrate	15236209I-060616/1	1
Caelo	Lactose monohydrate	15236213	2
Caelo	Lactose monohydrate	15236214	9
Caelo	Lactose monohydrate	15236215	4
Caelo	Lactose monohydrate	15236217	1
Caelo	Lactose monohydrate	15236220	5
Caelo	Lactose monohydrate	15236221	7
Caelo	Lactose monohydrate	1526201	1
Caelo	Lactose monohydrate	1565555	1
Caelo	Lactose monohydrate	16027701	6
Caelo	Lactose monohydrate	16027702	9
Caelo	Lactose monohydrate	16027703	6
Caelo	Lactose monohydrate	16027704	3
Caelo	Lactose monohydrate	16027705	1
Caelo	Lactose monohydrate	16027706	7
Caelo	Lactose monohydrate	16027707	2
Caelo	Lactose monohydrate	16027708	11
Caelo	Lactose monohydrate	16027726	1
Caelo	Lactose monohydrate	1606025-01	4
Caelo	Lactose monohydrate	1606025-1	1
Caelo	Lactose monohydrate	160913PJK01	1
Caelo	Lactose monohydrate	16091710	1
Caelo	Lactose monohydrate	162310206	1
Caelo	Lactose monohydrate	16231201	10
Caelo	Lactose monohydrate	16231202	20
Caelo	Lactose monohydrate	16231203	4
Caelo	Lactose monohydrate	16231206	7
Caelo	Lactose monohydrate	16231207	11
Caelo	Lactose monohydrate	16231208	5
Caelo	Lactose monohydrate	1623120803815470	1
Caelo	Lactose monohydrate	16231211	27
Caelo	Lactose monohydrate	16231212	10
Caelo	Lactose monohydrate	16231213	4
Caelo	Lactose monohydrate	162312135465	1
Caelo	Lactose monohydrate	16231214	5
Caelo	Lactose monohydrate	16231215	5
Caelo	Lactose monohydrate	16321202	1
Caelo	Lactose monohydrate	17011301	1
Caelo	Lactose monohydrate	1703019-01	3
Caelo	Lactose monohydrate	1703019-020	1
Caelo	Lactose monohydrate	17078302	11
Caelo	Lactose monohydrate	17078303	39
Caelo	Lactose monohydrate	17078303-20180619Ma2	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lactose monohydrate	17078306	11
Caelo	Lactose monohydrate	17078307	8
Caelo	Lactose monohydrate	17078312	25
Caelo	Lactose monohydrate	17321001	38
Caelo	Lactose monohydrate	173210016	1
Caelo	Lactose monohydrate	17321002	4
Caelo	Lactose monohydrate	17321004	9
Caelo	Lactose monohydrate	17321005	4
Caelo	Lactose monohydrate	17321006	1
Caelo	Lactose monohydrate	1733008	1
Caelo	Lactose monohydrate	17336001	1
Caelo	Lactose monohydrate	17336002	16
Caelo	Lactose monohydrate	17336005	12
Caelo	Lactose monohydrate	17336007	47
Caelo	Lactose monohydrate	17336008	20
Caelo	Lactose monohydrate	17336009	11
Caelo	Lactose monohydrate	17336013	20
Caelo	Lactose monohydrate	17336014	14
Caelo	Lactose monohydrate	1733609	1
Caelo	Lactose monohydrate	1802002-01	1
Caelo	Lactose monohydrate	18169016P-191115-2	1
Caelo	Lactose monohydrate	1818003	1
Caelo	Lactose monohydrate	18192001	1
Caelo	Lactose monohydrate	18196004	1
Caelo	Lactose monohydrate	18196023	2
Caelo	Lactose monohydrate	18198001	20
Caelo	Lactose monohydrate	18198002	6
Caelo	Lactose monohydrate	18198003	4
Caelo	Lactose monohydrate	18198005	1
Caelo	Lactose monohydrate	18198006	18
Caelo	Lactose monohydrate	18198007	24
Caelo	Lactose monohydrate	18198008	4
Caelo	Lactose monohydrate	18198009	1
Caelo	Lactose monohydrate	18198013	13
Caelo	Lactose monohydrate	18198014	11
Caelo	Lactose monohydrate	18198015	2
Caelo	Lactose monohydrate	18198016	24
Caelo	Lactose monohydrate	18198016P-191227-1	1
Caelo	Lactose monohydrate	18198017	6
Caelo	Lactose monohydrate	18198018	9
Caelo	Lactose monohydrate	18198023	22
Caelo	Lactose monohydrate	19137601	19
Caelo	Lactose monohydrate	19137601P-200303-1	1
Caelo	Lactose monohydrate	19137601P-200612-1	1
Caelo	Lactose monohydrate	19137602	7
Caelo	Lactose monohydrate	1922364001	1
Caelo	Lactose monohydrate	192346002	1
Caelo	Lactose monohydrate	192354015	1
Caelo	Lactose monohydrate	19236009	1
Caelo	Lactose monohydrate	192364001	6
Caelo	Lactose monohydrate	192364002	17
Caelo	Lactose monohydrate	192364003	13
Caelo	Lactose monohydrate	192364008	5
Caelo	Lactose monohydrate	192364009	14
Caelo	Lactose monohydrate	192364011	27
Caelo	Lactose monohydrate	192364012	18
Caelo	Lactose monohydrate	192364014	9
Caelo	Lactose monohydrate	192364015	16
Caelo	Lactose monohydrate	192364016	4
Caelo	Lactose monohydrate	19236403	30

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lactose monohydrate	2000400007	1
Caelo	Lactose monohydrate	20004200001	6
Caelo	Lactose monohydrate	20004200003	1
Caelo	Lactose monohydrate	20004200004	20
Caelo	Lactose monohydrate	20004200005	9
Caelo	Lactose monohydrate	20004200006	6
Caelo	Lactose monohydrate	20004200007	4
Caelo	Lactose monohydrate	20004200009	6
Caelo	Lactose monohydrate	2000420004	3
Caelo	Lactose monohydrate	2000420005	1
Caelo	Lactose monohydrate	20021411	1
Caelo	Lactose monohydrate	200415HJK02	1
Caelo	Lactose monohydrate	2011901	1
Caelo	Lactose monohydrate	201910028	1
Caelo	Lactose monohydrate	20223445	1
Caelo	Lactose monohydrate	2051702	1
Caelo	Lactose monohydrate	21001507003	13
Caelo	Lactose monohydrate	21001507004	13
Caelo	Lactose monohydrate	21001507005	4
Caelo	Lactose monohydrate	21001507008	2
Caelo	Lactose monohydrate	2100843006	1
Caelo	Lactose monohydrate	21071801	1
Caelo	Lactose monohydrate	21111813	1
Caelo	Lactose monohydrate	220000736007	1
Caelo	Lactose monohydrate	22000736001	4
Caelo	Lactose monohydrate	22000736003	4
Caelo	Lactose monohydrate	22000736005	7
Caelo	Lactose monohydrate	22000736006	6
Caelo	Lactose monohydrate	22000736007	8
Caelo	Lactose monohydrate	22000736008	4
Caelo	Lactose monohydrate	22000736009	3
Caelo	Lactose monohydrate	22000736010	4
Caelo	Lactose monohydrate	22000736011	4
Caelo	Lactose monohydrate	22000736012	2
Caelo	Lactose monohydrate	22000736017	1
Caelo	Lactose monohydrate	220401LM	1
Caelo	Lactose monohydrate	23001015002	1
Caelo	Lactose monohydrate	23001015003	3
Caelo	Lactose monohydrate	23001015007	1
Caelo	Lactose monohydrate	23002236003	1
Caelo	Lactose monohydrate	23051501	1
Caelo	Lactose monohydrate	23061504	1
Caelo	Lactose monohydrate	23101404	1
Caelo	Lactose monohydrate	24011405	1
Caelo	Lactose monohydrate	26061801	1
Caelo	Lactose monohydrate	26071401	1
Caelo	Lactose monohydrate	27101702	1
Caelo	Lactose monohydrate	2901312210	1
Caelo	Lactose monohydrate	30031503	1
Caelo	Lactose monohydrate	30081801	1
Caelo	Lactose monohydrate	30101201	1
Caelo	Lactose monohydrate	3031501	1
Caelo	Lactose monohydrate	3091405	1
Caelo	Lactose monohydrate	3121406	1
Caelo	Lactose monohydrate	3295	1
Caelo	Lactose monohydrate	3788916	1
Caelo	Lactose monohydrate	4313Q2210	1
Caelo	Lactose monohydrate	5011901	1
Caelo	Lactose monohydrate	5041702	1
Caelo	Lactose monohydrate	5061504	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lactose monohydrate	6091301	1
Caelo	Lactose monohydrate	6101702	1
Caelo	Lactose monohydrate	7031402	1
Caelo	Lactose monohydrate	7111402	1
Caelo	Lactose monohydrate	8021401	1
Caelo	Lactose monohydrate	8071501	1
Caelo	Lactose monohydrate	9051401	1
Caelo	Lactose monohydrate	9061803	1
Caelo	Lactose monohydrate	C1023	1
Caelo	Lactose monohydrate	s-100513-1	1
Caelo	Lactose monohydrate	Testmessung	1
Caeo/Noweda	Lactose monohydrate	1523204	1
Caesar & Loretz GmbH…	Lactose monohydrate	18198023	1
Caesar & Loretz GmbH…	Lactose monohydrate	18198002	2
Caesar & Loretz GmbH…	Lactose monohydrate	18198008	1
Caesar & Loretz GmbH…	Lactose monohydrate	18198014	2
Caesar & Loretz GmbH…	Lactose monohydrate	18198017	1
Caesar & Loretz GmbH…	Lactose monohydrate	19137601	3
Caesar & Loretz GmbH…	Lactose monohydrate	192364003	3
Caesar & Loretz GmbH…	Lactose monohydrate	192364012	1
Caesar & Loretz GmbH…	Lactose monohydrate	18198006	1
Caesar & Loretz GmbH…	Lactose monohydrate	192364008	1
Caesar & Loretz GmbH…	Lactose monohydrate	18198016	1
Caesar & Loretz GmbH/AHD	Lactose monohydrate	22000736007	1
Caesar & Loretz GmbH…	Lactose monohydrate	192364016	2
Caesar & Loretz GmbH…	Lactose monohydrate	22000736015	1
Caesar & Loretz GmbH…	Lactose monohydrate	18198023	1
Caesar & Loretz GmbH…	Lactose monohydrate	192364011	2
Caesar & Loretz GmbH/Gehe	Lactose monohydrate	18198002	2
Caesar & Loretz GmbH/Gehe	Lactose monohydrate	19137601	3
Caesar & Loretz GmbH/Gehe	Lactose monohydrate	192364002	1
Caesar & Loretz GmbH/Gehe	Lactose monohydrate	192364003	2
Caesar & Loretz GmbH/Gehe	Lactose monohydrate	192364014	2
Caesar & Loretz GmbH/Gehe	Lactose monohydrate	20004200001	1
Caesar & Loretz GmbH/Gehe	Lactose monohydrate	20004200005	1
Caesar & Loretz GmbH…	Lactose monohydrate	18198014	1
Caesar & Loretz GmbH…	Lactose monohydrate	20004200001	1
Caesar & Loretz GmbH…	Lactose monohydrate	20004200005	1
Caesar & Loretz GmbH…	Lactose monohydrate	20004200009	1
Caesar & Loretz GmbH…	Lactose monohydrate	21001507005	1
Caesar & Loretz GmbH…	Lactose monohydrate	22000736001	1
Caesar & Loretz GmbH…	Lactose monohydrate	22000736009	2
Caesar & Loretz GmbH…	Lactose monohydrate	22000736018	1
Caesar & Loretz GmbH…	Lactose monohydrate	18198007	1
Caesar & Loretz GmbH/Kehr	Lactose monohydrate	192364012	1
Caesar & Loretz GmbH…	Lactose monohydrate	18198022	3
Caesar & Loretz GmbH…	Lactose monohydrate	192364016	3
Caesar & Loretz GmbH/L10	Lactose monohydrate	192364009	1
Caesar & Loretz GmbH…	Lactose monohydrate	18198007	1
Caesar & Loretz GmbH…	Lactose monohydrate	21001507004	1
Caesar & Loretz GmbH…	Lactose monohydrate	22000736008	1
Caesar & Loretz GmbH…	Lactose monohydrate	18198017	2
Caesar & Loretz GmbH…	Lactose monohydrate	192364002	1
Caesar & Loretz GmbH…	Lactose monohydrate	19137601	2
Caesar & Loretz GmbH…	Lactose monohydrate	192364016	1
Caesar & Loretz GmbH…	Lactose monohydrate	20004200007	1
Caesar & Loretz GmbH…	Lactose monohydrate	20004200009	1
Caesar & Loretz GmbH	Lactose monohydrate	14140311	1
Caesar & Loretz GmbH	Lactose monohydrate	17321001	1
Caesar & Loretz GmbH	Lactose monohydrate	17336002	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Lactose monohydrate	17336007	3
Caesar & Loretz GmbH	Lactose monohydrate	17336009	1
Caesar & Loretz GmbH	Lactose monohydrate	17336013	3
Caesar & Loretz GmbH	Lactose monohydrate	18198001	7
Caesar & Loretz GmbH	Lactose monohydrate	18198002	11
Caesar & Loretz GmbH	Lactose monohydrate	18198003	3
Caesar & Loretz GmbH	Lactose monohydrate	18198006	4
Caesar & Loretz GmbH	Lactose monohydrate	18198007	6
Caesar & Loretz GmbH	Lactose monohydrate	18198008	3
Caesar & Loretz GmbH	Lactose monohydrate	18198013	2
Caesar & Loretz GmbH	Lactose monohydrate	18198014	5
Caesar & Loretz GmbH	Lactose monohydrate	18198016	7
Caesar & Loretz GmbH	Lactose monohydrate	18198018	1
Caesar & Loretz GmbH	Lactose monohydrate	18198023	4
Caesar & Loretz GmbH	Lactose monohydrate	19137601	3
Caesar & Loretz GmbH	Lactose monohydrate	192364001	1
Caesar & Loretz GmbH	Lactose monohydrate	192364002	6
Caesar & Loretz GmbH	Lactose monohydrate	192364003	2
Caesar & Loretz GmbH	Lactose monohydrate	192364008	2
Caesar & Loretz GmbH	Lactose monohydrate	192364009	4
Caesar & Loretz GmbH	Lactose monohydrate	192364011	10
Caesar & Loretz GmbH	Lactose monohydrate	192364012	8
Caesar & Loretz GmbH	Lactose monohydrate	192364014	10
Caesar & Loretz GmbH	Lactose monohydrate	192364015	7
Caesar & Loretz GmbH	Lactose monohydrate	192364016	1
Caesar & Loretz GmbH	Lactose monohydrate	19236403	3
Caesar & Loretz GmbH	Lactose monohydrate	20004200001	2
Caesar & Loretz GmbH	Lactose monohydrate	20004200004	8
Caesar & Loretz GmbH	Lactose monohydrate	20004200005	2
Caesar & Loretz GmbH	Lactose monohydrate	20004200006	2
Caesar & Loretz GmbH	Lactose monohydrate	20004200007	3
Caesar & Loretz GmbH	Lactose monohydrate	20004200009	2
Caesar & Loretz GmbH	Lactose monohydrate	21001507003	12
Caesar & Loretz GmbH	Lactose monohydrate	21001507004	1
Caesar & Loretz GmbH	Lactose monohydrate	21001507005	1
Caesar & Loretz GmbH	Lactose monohydrate	22000736001	7
Caesar & Loretz GmbH	Lactose monohydrate	22000736003	1
Caesar & Loretz GmbH	Lactose monohydrate	22000736005	6
Caesar & Loretz GmbH	Lactose monohydrate	22000736006	1
Caesar & Loretz GmbH	Lactose monohydrate	22000736007	1
Caesar & Loretz GmbH	Lactose monohydrate	22000736008	3
Caesar & Loretz GmbH	Lactose monohydrate	22000736009	1
Caesar & Loretz GmbH	Lactose monohydrate	22000736015	1
Caesar & Loretz GmbH	Lactose monohydrate	22000736016	2
Caesar & Loretz GmbH	Lactose monohydrate	22000736018	2
Caesar & Loretz GmbH	Lactose monohydrate	23001015001	1
Caesar & Loretz GmbH	Lactose monohydrate	23001015003	1
Caesar & Loretz Hilden	Lactose monohydrate	18198013	1
Caesar & Loretz Hilden	Lactose monohydrate	192364015	1
Caesar & Loretz Hilden	Lactose monohydrate	19236403	1
Caesar & Loretz/Geil...	Lactose monohydrate	18198006	1
Caesar & Loretz/Geil...	Lactose monohydrate	18198018	1
Caesar & Loretz/Geil...	Lactose monohydrate	192364009	1
Caesar & Loretz/Geil...	Lactose monohydrate	192364015	2
Caesar & Loretz/Noweda	Lactose monohydrate	15236204	1
Caesar & Loretz/Noweda	Lactose monohydrate	17336013	1
Caesar /phönix	Lactose monohydrate	13104901	2
Caesar Loretz	Lactose monohydrate	21001507004	1
Caesar u Loretz	Lactose monohydrate	1433520	1
Caesar u Loretz	Lactose monohydrate	16231202	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar u. Loretz	Lactose monohydrate	14025620	1
Caesar& Loretz GmbH	Lactose monohydrate	22000736005	1
Cealo	Lactose monohydrate	13104901	1
Cealo	Lactose monohydrate	16231202	1
cealo	Lactose monohydrate	1733002	1
cealo	Lactose monohydrate	21001507003	1
Celo/Kehr	Lactose monohydrate	16231213	2
cesar&lorentz/Phönix	Lactose monohydrate	12336815	1
Chiesi	Lactose monohydrate	16027708	1
Dr.Wolff/Noweda	Lactose monohydrate	14A30-B07-296182	1
Ebert u. Jacobi 1...	Lactose monohydrate	15236215	1
Edelweiss/Fiebig	Lactose monohydrate	279325290-0555	1
Edelweiss/Fiebig	Lactose monohydrate	293272062-0535	1
Edelweiss/Fiebig	Lactose monohydrate	294237160-1115	1
Edelweiss/Geibo	Lactose monohydrate	258710315-1203	1
Edelweiss	Lactose monohydrate	253292176-1124	1
Edelweiss	Lactose monohydrate	283256067-0930	1
Edelweiss	Lactose monohydrate	6886	1
Eigen	Lactose monohydrate	129I20	1
Eigen	Lactose monohydrate	129I21	1
Eigenherstellung/ De...	Lactose monohydrate	10112101	1
Eigenherstellung	Lactose monohydrate	110913HJK01	1
Eigenherstellung	Lactose monohydrate	40113HJK01	1
Eigenherstellung	Lactose monohydrate	40815HMS01	1
Eigenherstellung	Lactose monohydrate	60814HSA01	1
Eigenherstellung	Lactose monohydrate	70113HML01	1
EuRho	Lactose monohydrate	1112020-01	1
EuRho	Lactose monohydrate	1112020-02	2
EuRho	Lactose monohydrate	1301028-01	1
EuRho	Lactose monohydrate	1501017-01	1
EuRho	Lactose monohydrate	1509030-02	1
EuRho	Lactose monohydrate	1606025-02	1
EuRho	Lactose monohydrate	170301901	3
Eurho	Lactose monohydrate	1802002-01	2
EuRho	Lactose monohydrate	1909014-01	2
Euro OCT	Lactose monohydrate	1401003-01	3
Euro OTC	Lactose monohydrate	1013Q-02210	1
Euro OTC	Lactose monohydrate	110602202	1
Euro OTC	Lactose monohydrate	1112020-01	2
Euro OTC	Lactose monohydrate	1112020-02	4
Euro OTC	Lactose monohydrate	130102801	1
Euro OTC	Lactose monohydrate	1301028-01	8
Euro OTC	Lactose monohydrate	1301028-02	12
Euro OTC	Lactose monohydrate	1301028-03	2
Euro OTC	Lactose monohydrate	1401003	1
Euro OTC	Lactose monohydrate	1401003-01	10
Euro OTC	Lactose monohydrate	140-1003-01	1
Euro OTC	Lactose monohydrate	140100302	1
Euro OTC	Lactose monohydrate	1401003-02	7
Euro OTC	Lactose monohydrate	14025604	2
Euro OTC	Lactose monohydrate	14025616	2
Euro OTC	Lactose monohydrate	15010	1
Euro OTC	Lactose monohydrate	150101701	1
Euro OTC	Lactose monohydrate	1501017-01	11
Euro OTC	Lactose monohydrate	1501017-02	1
Euro OTC	Lactose monohydrate	1509030-01	7
Euro OTC	Lactose monohydrate	150903002	1
Euro OTC	Lactose monohydrate	1509030-02	7
Euro OTC	Lactose monohydrate	15090-30-02	1
Euro OTC	Lactose monohydrate	160602501	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Lactose monohydrate	1606025-01	30
Euro OTC	Lactose monohydrate	1606025-02	4
Euro OTC	Lactose monohydrate	1703019-01	6
Euro OTC	Lactose monohydrate	1703019-02	6
Euro OTC	Lactose monohydrate	17A11-B01-334251	1
Euro OTC	Lactose monohydrate	180200201	2
Euro OTC	Lactose monohydrate	1802002-01	12
Euro OTC	Lactose monohydrate	1802002-02	1
Euro OTC	Lactose monohydrate	1802002-03	1
Euro OTC	Lactose monohydrate	180202-01	1
Euro OTC	Lactose monohydrate	18082014A	1
Euro OTC	Lactose monohydrate	1812008-01	14
Euro OTC	Lactose monohydrate	1812008-02	8
Euro OTC	Lactose monohydrate	1812008-03	2
Euro OTC	Lactose monohydrate	1909014-01	23
Euro OTC	Lactose monohydrate	1909014-02	2
Euro OTC	Lactose monohydrate	2005026	1
Euro OTC	Lactose monohydrate	200502601	2
Euro OTC	Lactose monohydrate	2005026-01	12
Euro OTC	Lactose monohydrate	2005026-0108597888	1
Euro OTC	Lactose monohydrate	2005026-02	2
Euro OTC	Lactose monohydrate	20052026-02	1
Euro OTC	Lactose monohydrate	2201013-01	5
Euro OTC	Lactose monohydrate	2208008-01	3
Euro OTC	Lactose monohydrate	31102013A	1
Euro OTC	Lactose monohydrate	3215A-02210	1
Euro OTC	Lactose monohydrate	5123	1
Euro OTC	Lactose monohydrate	L101852618	1
Euro OTC	Lactose monohydrate	L101854417A545	1
Euro OTC	Lactose monohydrate	L1237A4172	2
Euro OTC	Lactose monohydrate	UP250171017	1
Euro/Phönix	Lactose monohydrate	1802002-01	1
Euro/Phönix	Lactose monohydrate	1909014-01	2
Euroo/Phoenix	Lactose monohydrate	1401003-02	1
Europ Ots Pharma	Lactose monohydrate	1301028-02	3
Europ Ots Pharma	Lactose monohydrate	1401003-02	1
Europharm/Otto	Lactose monohydrate	1106022-01	1
Fagron	Lactose monohydrate	10726158	1
Fagron	Lactose monohydrate	10751120	1
Fagron	Lactose monohydrate	11C29-N06	1
Fagron	Lactose monohydrate	11L22-N03	1
Fagron	Lactose monohydrate	12/23-B02-287554	1
Fagron	Lactose monohydrate	12C09-N04	1
Fagron	Lactose monohydrate	12C26-N05	1
Fagron	Lactose monohydrate	12G27-N02	5
Fagron	Lactose monohydrate	13/23-B02-287554	1
Fagron	Lactose monohydrate	1301C005-278129	2
Fagron	Lactose monohydrate	1301C006-278128	6
Fagron	Lactose monohydrate	1301C007-278131	1
Fagron	Lactose monohydrate	1303C001	1
Fagron	Lactose monohydrate	1303C001-280388	1
Fagron	Lactose monohydrate	1303C002-280398	1
Fagron	Lactose monohydrate	1303C003	1
Fagron	Lactose monohydrate	1303C003-280390	1
Fagron	Lactose monohydrate	13E23-B01	2
Fagron	Lactose monohydrate	13E23-B01-283332	2
Fagron	Lactose monohydrate	13E23-B01-283334	1
Fagron	Lactose monohydrate	13I23-B03	4
Fagron	Lactose monohydrate	13I23-B03-287414	1
Fagron	Lactose monohydrate	13I23-B03-291115	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Lactose monohydrate	13I23-B03-291116	1
Fagron	Lactose monohydrate	13J23-B03-291114	1
Fagron	Lactose monohydrate	14140312	1
Fagron	Lactose monohydrate	14333518	1
Fagron	Lactose monohydrate	14333525	1
Fagron	Lactose monohydrate	14A30-B07	2
Fagron	Lactose monohydrate	14A30-B07-296182	2
Fagron	Lactose monohydrate	14H27-B01-305666	1
Fagron	Lactose monohydrate	14H27-B02	1
Fagron	Lactose monohydrate	14H27-B02-302033	2
Fagron	Lactose monohydrate	15A19-B06	4
Fagron	Lactose monohydrate	15A19-B06-303437	3
Fagron	Lactose monohydrate	15A19-B06-303439	8
Fagron	Lactose monohydrate	15H14-B03-314451	3
Fagron	Lactose monohydrate	16231215	1
Fagron	Lactose monohydrate	1623123	1
Fagron	Lactose monohydrate	16A05-B03	1
Fagron	Lactose monohydrate	17078302	1
Fagron	Lactose monohydrate	17321001	1
Fagron	Lactose monohydrate	17336007	2
Fagron	Lactose monohydrate	1802002-01	1
Fagron	Lactose monohydrate	18B15-B06-353917	1
Fagron	Lactose monohydrate	18B15-B06-35917	1
Fagron	Lactose monohydrate	2005026-02	2
Fagron	Lactose monohydrate	282567/0	1
Fiebig	Lactose monohydrate	19236403	2
Finteler Apotheke	Lactose monohydrate	16231211	1
Fragon	Lactose monohydrate	10706040	1
Gatt-Koller / Phoenix	Lactose monohydrate	5580/12120813	2
Gatt-Koller	Lactose monohydrate	1702456	1
GEHE am 17.06.2014	Lactose monohydrate	13299108	1
Gehe/Caesar & Loretz GmbH	Lactose monohydrate	18198002	3
Gehe	Lactose monohydrate	1112020-01	1
Gehe	Lactose monohydrate	1112020-02	3
Gehe	Lactose monohydrate	1301028-02	2
Gehe	Lactose monohydrate	14025620	1
Gehe	Lactose monohydrate	14333502	1
gehe	Lactose monohydrate	16231211	1
Gehe	Lactose monohydrate	16231211	1
Gehe	Lactose monohydrate	17078303	2
GEHE	Lactose monohydrate	17321001	1
GEHE	Lactose monohydrate	17321006	2
GEHE	Lactose monohydrate	17336005	1
GEHE	Lactose monohydrate	17336008	1
GEHE	Lactose monohydrate	17336014	2
Gehe	Lactose monohydrate	1802002-01	1
Gehe	Lactose monohydrate	18198001	1
GEHE	Lactose monohydrate	18198008	2
Gehe	Lactose monohydrate	18198014	1
GEHE	Lactose monohydrate	18198017	1
Gehe	Lactose monohydrate	2300101004	1
Gehe	Lactose monohydrate	23001015004	2
Geilenkirchen	Lactose monohydrate	17336014	1
Geilenkirchen	Lactose monohydrate	18198002	3
Geilenkirchen	Lactose monohydrate	192364003	2
Geilenkirchen	Lactose monohydrate	192364016	4
Geilenkirchen	Lactose monohydrate	21001507005	2
Geilenkirchen	Lactose monohydrate	22000736006	1
Jenne	Lactose monohydrate	192364002	1
Jenne	Lactose monohydrate	23002236003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Kehr 15.09.2020	Lactose monohydrate	192364011	1
Kehr	Lactose monohydrate	17321004	1
Kehr	Lactose monohydrate	22000736008	1
Kehr	Lactose monohydrate	22000736018	1
Kehr	Lactose monohydrate	23001015007	1
kölln GmbH	Lactose monohydrate	305749041-1056	1
Kölln GmbH	Lactose monohydrate	316349	1
L10	Lactose monohydrate	1606025-01	1
L12	Lactose monohydrate	1703019-01	1
L30	Lactose monohydrate	1703019-02	1
L30	Lactose monohydrate	1802002-01	1
Maros/Phoenix	Lactose monohydrate	192364012	1
Max Jenne	Lactose monohydrate	23003217001	1
Nachprüfung	Lactose monohydrate	3712Q-02210	1
Noweda/ Caesar&Loretz	Lactose monohydrate	12336815	1
Noweda	Lactose monohydrate	14025601	1
Noweda	Lactose monohydrate	16231215	1
Noweda	Lactose monohydrate	1703019-01	1
Noweda	Lactose monohydrate	1703019-02	1
Noweda	Lactose monohydrate	17078303	1
Noweda	Lactose monohydrate	1802002-01	3
Noweda	Lactose monohydrate	1802002-02	1
Noweda	Lactose monohydrate	1812008-02	1
Noweda	Lactose monohydrate	1812008-03	1
Noweda	Lactose monohydrate	1909014-01	2
Noweda	Lactose monohydrate	192364014	1
Noweda	Lactose monohydrate	21001507003	1
Noweda	Lactose monohydrate	22000736011	3
Noweda	Lactose monohydrate	22000736015	1
Noweda	Lactose monohydrate	23001015001	1
Noweda	Lactose monohydrate	23001015007	1
Noweda	Lactose monohydrate	L101854417A545	1
Otto Fischar GmbH	Lactose monohydrate	16231202	1
Otto Geilenkirchen GmbH	Lactose monohydrate	18198007	2
otz pharma	Lactose monohydrate	130102802	1
Peter Kölln GmbH & C…	Lactose monohydrate	256549266-0636	1
Peter Kölln	Lactose monohydrate	229719241-0640	1
pharmachem	Lactose monohydrate	15236208	1
Phoenix 19.03.2014	Lactose monohydrate	13104909	1
Phoenix 19.1.2019	Lactose monohydrate	18198001	1
Phoenix 30.04.2014	Lactose monohydrate	13E23-B01-283332	1
Phoenix 7.11.19	Lactose monohydrate	1802002-01	3
Phoenix	Lactose monohydrate	1404PLV-1928	4
Phoenix	Lactose monohydrate	15A19-B06	3
Phoenix	Lactose monohydrate	17321001	1
Phoenix	Lactose monohydrate	17336013	1
Phoenix	Lactose monohydrate	1909014-01	1
Phoenix	Lactose monohydrate	23003217001	1
Phoenix	Lactose monohydrate	3194	1
Phönix 17.05.2019	Lactose monohydrate	1812008-01	3
Phönix 28.08.2019	Lactose monohydrate	1812008-02	2
Phönix	Lactose monohydrate	12336815	1
Phönix	Lactose monohydrate	13299102	2
Phönix	Lactose monohydrate	14025616	1
Phönix	Lactose monohydrate	16027701	1
phönix	Lactose monohydrate	16231202	1
PHÖNIX	Lactose monohydrate	16A05-B03-322529	2
Phönix	Lactose monohydrate	17321001	1
Phönix	Lactose monohydrate	181200801	1
Phönix	Lactose monohydrate	18198001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Lactose monohydrate	18198007	1
Phönix	Lactose monohydrate	192364012	1
phönix	Lactose monohydrate	22000736005	1
Rondell Apotheke	Lactose monohydrate	1509030-01	2
Sana/Hanse	Lactose monohydrate	23003217003	1
Sanacorp,05.04.17, 5,96EUR	Lactose monohydrate	16231202	1
Sanacorp	Lactose monohydrate	12336815	1
Sanacorp	Lactose monohydrate	13104901	1
Sanacorp	Lactose monohydrate	13104909	1
Sanacorp	Lactose monohydrate	13299102	1
Sanacorp	Lactose monohydrate	13299108	1
Sanacorp	Lactose monohydrate	14025620	1
Sanacorp	Lactose monohydrate	14333509	1
Sanacorp	Lactose monohydrate	14333518	1
Sanacorp	Lactose monohydrate	16231215	1
Sanacorp	Lactose monohydrate	17078303	1
Sanacorp	Lactose monohydrate	17078306	1
Sanacorp	Lactose monohydrate	17078312	1
Sanacorp	Lactose monohydrate	17321001	1
Sanacorp	Lactose monohydrate	17321004	1
Sanacorp	Lactose monohydrate	1802002	1
Sanacorp	Lactose monohydrate	18198016	1
Sanacorp	Lactose monohydrate	18198017	3
Sanacorp	Lactose monohydrate	192364002	1
Sanacorp	Lactose monohydrate	22000736005	2
sanacorp	Lactose monohydrate	22000736008	1
Sanacorp	Lactose monohydrate	22000736017	1
Sanacorp	Lactose monohydrate	23001015004	1
Sanacorp	Lactose monohydrate	23001015007	1
Sanacorp	Lactose monohydrate	23002236003	1
Sanacorp	Lactose monohydrate	274600148-0724	1
Sanacorp	Lactose monohydrate	274600148-0726	1
Sanacorp	Lactose monohydrate	283259077-1133	2
Sanacorp	Lactose monohydrate	283259077-1214	1
Sanacorp	Lactose monohydrate	285739172-1842	2
Sanacorp	Lactose monohydrate	285739172-1852	2
Sanacorp	Lactose monohydrate	285739172-1853	1
schubert / Phoenix	Lactose monohydrate	1334PLV-1775	1
siehe Protokoll	Lactose monohydrate	1606025-01	1
Spangropharm	Lactose monohydrate	91444379	1
vdl	Lactose monohydrate	1112020-01	2
Zentralapotheke Wetzlar	Lactose monohydrate	213L20	1

- 233 602 spectra from 1515 *Apo-Ident* customers from a total of 48 750 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Lactose monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lactose monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	430	0	152 532
Type B	0	620	0	201 464
Type C	0	2459	6	233 602

The substance/substance group *Lactose monohydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6047 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0323 %)
Type C	100.0000 % (> 99.9007 %)	99.7566 % (> 99.6349 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20685	22460	5.62	65.73
21525	22460	6.99	63.19
21526	22460	8.27	62.10
21527	22460	6.64	62.48
21528	22460	7.24	63.06
21529	22460	5.46	64.97
21935	21935	0.00	71.20
22460	22460	0.00	69.98
22701	22701	0.00	69.40
24929	24929	0.00	72.48

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**L-alanine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	23776-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

L-alanine; Alaninum

Special notes

When selecting the *L-alanine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
L-alanine	3	1	1

Second-stage model

For differentiation of the substance/substance group *L-alanine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *L-alanine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Glycine	70.74	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *L-alanine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *L-alanine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	L-alanine	1710009	23776	40	20171018*
Euro OTC	L-alanine	2008025	25396	40	20200910*
Fagron	L-alanine	23F28-B02-230972	26905	40	20230721

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 120 spectra of 3 reference samples from the substance/substance group *L-alanine*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 842 spectra from a total of 2839 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 60 spectra of 2 reference samples from the substance/substance group *L-alanine*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	L-alanine	1601033-01	23905	40
Fagron	L-alanine	23F28-B02-230972	26905SI†	20

- 202 024 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *L-alanine*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	L-alanine	2008025-01	2

- 236 065 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *L-alanine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *L-alanine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	120	0	152 842
Type B	0	60	0	202 024
Type C	0	2	0	236 065

The substance/substance group *L-alanine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.9013 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23776	23776	0.00	175.60
25396	25396	0.00	158.45
26905	25396	17.13	168.92

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Leucine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20970-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Leucine; L-Leucine; Leucinum

Special notes

When selecting the *Leucine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Leucine	6	7	5

Second-stage model

For differentiation of the substance/substance group *Leucine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Leucine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Isoleucine	54.20	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Leucine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Leucine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Leucine	1302013-01	21612	60	20130320
Euro OTC	Leucine	1601032	22380	40	20160308*
Euro OTC	Leucine	2004006	25165	40	20200507*
Euro OTC	Leucine	2011008	25467	40	20201204*
Fagron	Leucine	13J09-N03	20970	40	1402431
Fagron	Leucine	15D09-B06-322249	23199	40	20151030

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 6 reference samples from the substance/substance group *Leucine*. These samples

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 330 spectra of 10 reference samples from the substance/substance group *Leucine*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Leucine	1708010	23607	40
Euro OTC	Leucine	1901008	24473	40
Euro OTC	Leucine	2203014	26041	40
Euro OTC	Leucine	2302005	26646	40
Euro OTC	Leucine	2401011	27144	40
Euro OTC	Leucine	2404015	27292	40
Fagron	Leucine	23F15-B10-231014	26907	40
Euro OTC	Leucine	2203014	26041SI	10
Euro OTC	Leucine	2302005	26646SI	20
Fagron	Leucine	23F15-B10-231014	26907SI	20

- 201 754 spectra from a total of 4038 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Leucine*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Leucine	1312032-01	1
Euro OTC	Leucine	1708010-01	2
Euro OTC	Leucine	700113	1
Fagron	Leucine	20J15-B02-202893	1
Fargon	Leucine	8160410903	1

- 236 061 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Leucine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Leucine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	330	0	201 754
Type C	0	6	0	236 061

The substance/substance group *Leucine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.1818 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20970	20970	0.00	105.92
21612	25165	17.94	110.61

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22380	22380	0.00	111.28
23199	25467	12.39	115.70
25165	25165	0.00	115.04
25467	25467	0.00	114.43

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Levocarnitine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20357-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Levocarnitine; Levocarnitinum

Special notes

When selecting the *Levocarnitine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Levocarnitine	7	9	20

Second-stage model

For differentiation of the substance/substance group *Levocarnitine* the following second-stage model is used:

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Levocarnitine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cystine	89.95	–
⋮	⋮	⋮
Valine	>50	80.66
Oxybutynin hydrochloride	>50	138.67
Capsaicin	>50	181.45
Sodium citrate	>50	192.32
Prednicarbate	>50	242.22
Cyproterone acetate	>50	257.34
Pyridoxal-5-phosphate	>50	276.98
Methoxsalen	>50	313.92
Alfatradiol	>50	441.44
Quinine hydrochloride dihydrate	>50	458.90
Amitriptyline hydrochloride	>50	468.12
Tetracaine	>50	471.37
Norethisterone acetate	>50	491.07
Ciprofloxacin hydrochloride	>50	542.57
Heparin sodium	>50	839.92
Triclosan	>50	1346.42
Amifampridine	>50	2252.13
Sucrose	>50	2278.79

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Levocarnitine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Levocarnitine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Levocarnitine	1210029-01	20809	40	20121130
Euro OTC	Levocarnitine	2007040-01	25606	40	20201215

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Levocarnitine	2104006	25681	40	20210423*
Fagron	Levocarnitine	12H10-N07	20818	40	20120830
Fagron	Levocarnitine	14A20-B11-290728	21790	60	AR-15-FG-016322-01
Fagron	Levocarnitine	14A20-B11-290728	21968	60	AR-16-FG-005969-01
Fagron	Levocarnitine	15L04-B05-319229	23194	40	AR-17-FG-012937-01
Fagron	Levocarnitine	16L06-B03-338285	23919	40	20161227

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 8 reference samples from the substance/substance group *Levocarnitine*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 602 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 440 spectra of 12 reference samples from the substance/substance group *Levocarnitine*.

- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Levocarnitine	1303027-02	21648	60
Euro OTC	Levocarnitine	2203025	26087	40
Euro OTC	Levocarnitine	2301027	26532	40
Euro OTC	Levocarnitine	2406011	27344	40
Euro OTC	Levocarnitine	2410001	27456	40
Fagron	Levocarnitine	16F20-B01-326616	23402	40
Fagron	Levocarnitine	17K23-B01-345633	24009	40
Fagron	Levocarnitine	22B02-B10-220587	26164	40
Fagron	Levocarnitine	24A05-B04-235963	27169	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Levocarnitine	2203025	26087SI	20
Euro OTC	Levocarnitine	2301027	26532SI	20
Fagron	Levocarnitine	22B02-B10-220587	26164SI	20

- 201 644 spectra from a total of 4036 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 38 spectra from 12 *Apo-Ident* customers from 21 batches from the substance/substance group *Levocarnitine*.
- Among them are spectra of independent samples from 20 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Levocarnitine	2301027-01	1
Denk	Levocarnitine	A04217	1
EuRho	Levocarnitine	2007040-01	1
Euro OTC	Levocarnitine	1303027	1
Euro OTC	Levocarnitine	1705006-01	1
Euro OTC	Levocarnitine	1808027-01	1
Euro OTC	Levocarnitine	200402401	1
Euro OTC	Levocarnitine	2007040-01	3
Euro OTC	Levocarnitine	2203025-01	1
Euro OTC	Levocarnitine	L1608038-01	2
Euro OTC	Levocarnitine	L1705006-01	1
Euro OTC	Levocarnitine	L1801028-02	1
Euro OTC	Levocarnitine	L180802701	1
Fagron	Levocarnitine	13111701	1
Fagron	Levocarnitine	13G19-N12	2
Fagron	Levocarnitine	17K23-B01-346658	1
Fagron	Levocarnitine	19K08-F04	7
Fagron	Levocarnitine	19K08F04367748	2
Fagron	Levocarnitine	20B21-F01-370194	1
Fagron	Levocarnitine	20B21-F04	6
Fagron	Levocarnitine	9041504	1
Fagron	Levocarnitine	LC191017	1

- 236 029 spectra from 1515 *Apo-Ident* customers from a total of 49 238 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Levocarnitine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

all relevant spectra of the various substances were compared with *Levocarnitine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	440	0	201 644
Type C	0	38	0	236 029

The substance/substance group *Levocarnitine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6364 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 84.2105 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20809	21790	29.34	194.35
20818	23194	30.32	207.28
21790	21790	0.00	197.76
21968	21968	0.00	186.62
23194	23194	0.00	184.75
23919	25681	24.29	193.77
25606	23194	29.79	210.38
25681	25681	0.00	170.75

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Levothyroxin sodium**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21708-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Levothyroxin sodium; Levothyroxinum natrii

Special notes

When selecting the *Levothyroxin sodium* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Levothyroxin sodium	6	4	3

Second-stage model

For differentiation of the substance/substance group *Levothyroxin sodium* the following second-stage model is used:

- Submodel 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Levothyroxin sodium* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Eosin Y	74.85	33.58
⋮	⋮	⋮
Dequalinium chloride	>50	71.18
Tannin	>50	121.78
Oxytetracycline hydrochloride	>50	166.70
Acetylsalicylic acid	>50	477.75
Dithranol	>50	561.99
Sodium salicylate	>50	635.67
Benzoic acid	>50	920.19

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Levothyroxin sodium* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Levothyroxin sodium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Levothyroxin sodium	14E28-B05-298322	21708	30	1506426
Fagron	Levothyroxin sodium	14E28-B05-298322	21708SI	47	1506426
Fagron	Levothyroxin sodium	14E28-B05-306102	21820	60	20140915
Fagron	Levothyroxin sodium	14E28-B05-306102	21820SI	53	20140915
Fagron	Levothyroxin sodium	18G27-B02-352032	24286	40	20180822
Fagron	Levothyroxin sodium	20D01-F05-370575	25438	40	2110083
Fagron	Levothyroxin sodium	20D01-F05-370575	25438SI	39	2110083
Fagron	Levothyroxin sodium	20J01-F07-374963	25740	40	20201112
Fagron	Levothyroxin sodium	20J01-F07-374963	26080	40	20201112
Fagron	Levothyroxin sodium	20J01-F07-374963	26080SI	40	20201112
Fagron	Levothyroxin sodium	22C02-B03-223067	26333	40	20220613
Fagron	Levothyroxin sodium	22C02-B03-223067	26333SI	37	20220613

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 506 spectra of 12 reference samples from the substance/substance group *Levothyroxin sodium*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 456 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 364 spectra of 10 reference samples from the substance/substance group *Levothyroxin sodium*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Levothyroxin sodium	16G25-B99-329080	23191	40
Fagron	Levothyroxin sodium	17J10-B05-348764	24176	40
Fagron	Levothyroxin sodium	21I10-B10-217006	26068	40
Fagron	Levothyroxin sodium	23D29-B02-227893	27066	40
Fagron	Levothyroxin sodium	16G25-B99-329080	23191SI	24
Fagron	Levothyroxin sodium	17J10-B05-348764	24176SI	30
Fagron	Levothyroxin sodium	18G27-B02-352032	24286SI†	32
Fagron	Levothyroxin sodium	20J01-F07-374963	25740SI†	40
Fagron	Levothyroxin sodium	21I10-B10-217006	26068SI	40
Fagron	Levothyroxin sodium	23D29-B02-227893	27066SI	38

- 201 720 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 22 spectra from 7 *Apo-Ident* customers from 5 batches from the substance/substance group *Levothyroxin sodium*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Levothyroxin sodium	17J10-B05-345570	1
Fagron	Levothyroxin sodium	16G25-B99-324827	17
Fagron	Levothyroxin sodium	20D01-F05-370575	2
Fagron	Levothyroxin sodium	20J01-F07-374963	1
Fagron	Levothyroxin sodium	21/10-B10-217006	1

- 236 045 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Levothyroxin sodium* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Levothyroxin sodium* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	506	0	152 456
Type B	0	364	0	201 720
Type C	0	22	0	236 045

The substance/substance group *Levothyroxin sodium* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8142 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.3516 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 72.7273 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21708	21708	0.00	67.11
21820	25438	37.98	78.20
24286	25438	15.24	82.52
25438	25438	0.00	89.05
25740	25438	5.49	85.98
26080	25438	7.64	88.12
26333	25438	8.68	82.41

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Lidocaine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20942-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lidocaine; Lidocainum

Special notes

When selecting the *Lidocaine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Lidocaine	9	14	389

Second-stage model

For differentiation of the substance/substance group *Lidocaine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Lidocaine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Menthol	126.55	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Lidocaine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Lidocaine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Lidocaine	13352411	21673	60	20131115
Caelo	Lidocaine	180444	24031	40	20180419*
Euro OTC	Lidocaine	1310023-01	21640	60	20131118
Euro OTC	Lidocaine	1612021	22984	40	20170206*
Euro OTC	Lidocaine	1911005	24928	40	20191129*
Euro OTC	Lidocaine	2101035	25533	40	20210304*
Euro OTC	Lidocaine	2304015	26654	40	20230510*
Euro OTC	Lidocaine	2304015	26654SI	20	20230510*
Fagron	Lidocaine	13H05-N05	20942	40	1401378
Fagron	Lidocaine	16F21-B06-327232	23019	40	20160728

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 420 spectra of 10 reference samples from the substance/substance group *Lidocaine*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 542 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 600 spectra of 16 reference samples from the substance/substance group *Lidocaine*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Lidocaine	162895	22768	40
Caelo	Lidocaine	171831	23632	40
Caelo	Lidocaine	190545	24530	40
Caelo	Lidocaine	22000398	26736	40
Caelo	Lidocaine	23002079	26964	40
Euro OTC	Lidocaine	1603027	22526	40
Euro OTC	Lidocaine	1801032	23960	40
Euro OTC	Lidocaine	1902003	24475	40
Euro OTC	Lidocaine	1905004	24610	40
Euro OTC	Lidocaine	1908005	24847	40
Euro OTC	Lidocaine	2006013	25244	40
Euro OTC	Lidocaine	2206002	26230	40
Euro OTC	Lidocaine	2310020	27075	40
Fagron	Lidocaine	22C15-B17-216737	26134	40
Euro OTC	Lidocaine	2206002	26230SI	20
Fagron	Lidocaine	22C15-B17-216737	26134SI	20

- 201 484 spectra from a total of 4031 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1728 spectra from 697 *Apo-Ident* customers from 418 batches from the substance/substance group *Lidocaine*.

- Among them are spectra of independent samples from 389 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Lidocaine	1908005-01	1
	Lidocaine	20003343016	4
	Lidocaine	20H13-F04-373497	1
	Lidocaine	20L11-F01-376356	1
	Lidocaine	22000398003	2
	Lidocaine	22000398004	1
	Lidocaine	22000398010	1
	Lidocaine	22000398011	9
	Lidocaine	22000398013	5
	Lidocaine	22000398015	2
	Lidocaine	22000398016	7
	Lidocaine	2206002-01	1
	Lidocaine	22C15-B17	1
	Lidocaine	22C15-B17-216737	4
	Lidocaine	22C15-B17-216738	2
	Lidocaine	22C15-B17-216739	5
	Lidocaine	22c15-b17-225236	1
	Lidocaine	22C15-B17-225236	2
	Lidocaine	23002079001	1
	Lidocaine	2304015-01	1
	Lidocaine	23D25-B10-230220	1
	Lidocaine	23D25-B10-230226	2
	Lidocaine	B10-2302201	2
	Lidocaine	B17-2137307	1
	Lidocaine	LDB/722005	2
AHD	Lidocaine	15332314	1
AHD	Lidocaine	19054506	1
AHD	Lidocaine	22C15B17-225236	1
Alliance Healthcare	Lidocaine	19F27-B01-363501	1
Alliance Healthcare	Lidocaine	19F27-B01-363506	1
Alliance Healthcare	Lidocaine	20L11-F01-376356	1
Alliance Healthcare	Lidocaine	22C15-B17-225236	1
Alliance	Lidocaine	15H27-B07-318310	1
Alliance	Lidocaine	22000398010	1
Alliance	Lidocaine	22C15-B17-216737	1
Allianz Healthcare	Lidocaine	8565960	1
Alte Apotheke	Lidocaine	16A28B06-321297	1
Anzag	Lidocaine	12E30-N10	1
Audor Pharma	Lidocaine	1911005-01	1
Cae	Lidocaine	20003343010	1
Caelo	Lidocaine	11K17-N03	1
Caelo	Lidocaine	12163802	2
Caelo	Lidocaine	12163803	3
Caelo	Lidocaine	12163804	2
Caelo	Lidocaine	12163810	1
Caelo	Lidocaine	12163811	4
Caelo	Lidocaine	12163813	5
Caelo	Lidocaine	122294405	1
Caelo	Lidocaine	12294405	2
Caelo	Lidocaine	12294408	2
Caelo	Lidocaine	12294412	10
Caelo	Lidocaine	12294413	1
Caelo	Lidocaine	133522408	1
Caelo	Lidocaine	133524	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lidocaine	13352403	1
Caelo	Lidocaine	13352405	1
Caelo	Lidocaine	13352406	1
Caelo	Lidocaine	13352408	9
Caelo	Lidocaine	13352411	6
Caelo	Lidocaine	13352413	3
Caelo	Lidocaine	13352414	2
Caelo	Lidocaine	13352415	3
Caelo	Lidocaine	13J30-B02-292221	1
Caelo	Lidocaine	14299301	2
Caelo	Lidocaine	14299303	2
Caelo	Lidocaine	14299305	2
Caelo	Lidocaine	1512003	1
Caelo	Lidocaine	15212001	2
Caelo	Lidocaine	15212002	4
Caelo	Lidocaine	15212003	3
Caelo	Lidocaine	15332302	5
Caelo	Lidocaine	15332303	1
Caelo	Lidocaine	15332305	2
Caelo	Lidocaine	15332306	3
Caelo	Lidocaine	15332309	2
Caelo	Lidocaine	15332310	4
Caelo	Lidocaine	15332314	2
Caelo	Lidocaine	15A15-B01-304284	3
Caelo	Lidocaine	15D23-B08	1
Caelo	Lidocaine	15H27-B07-318310	1
Caelo	Lidocaine	15H-B07-318310	1
Caelo	Lidocaine	16087702	1
Caelo	Lidocaine	16087703	1
Caelo	Lidocaine	16087704	8
Caelo	Lidocaine	16087707	9
Caelo	Lidocaine	16087708	1
Caelo	Lidocaine	16087709	1
Caelo	Lidocaine	16087710	3
Caelo	Lidocaine	16087711	10
Caelo	Lidocaine	16087712	7
Caelo	Lidocaine	1608774	1
Caelo	Lidocaine	160877708	1
Caelo	Lidocaine	1612021-04	1
Caelo	Lidocaine	16289502	11
Caelo	Lidocaine	16289503	10
Caelo	Lidocaine	16289504	2
Caelo	Lidocaine	16289507	2
Caelo	Lidocaine	16289508	19
Caelo	Lidocaine	1629508	1
Caelo	Lidocaine	16A28-B06-320059	1
Caelo	Lidocaine	16F21-806-333787	1
Caelo	Lidocaine	16F21-B06-323670	1
Caelo	Lidocaine	16F21-B06-326631	1
Caelo	Lidocaine	16F21-B06-328421	3
Caelo	Lidocaine	1718308	1
Caelo	Lidocaine	17183102	3
Caelo	Lidocaine	17183103	8
Caelo	Lidocaine	17183105	1
Caelo	Lidocaine	17183106	1
Caelo	Lidocaine	17183108	8
Caelo	Lidocaine	17183109	9
Caelo	Lidocaine	17348502	6
Caelo	Lidocaine	17348503	15
Caelo	Lidocaine	17348503P-190516-5	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lidocaine	1783109	2
Caelo	Lidocaine	17G03-B08	1
Caelo	Lidocaine	17G03B08338286	1
Caelo	Lidocaine	17G03-B08-341306	3
Caelo	Lidocaine	17G03B08341308	1
Caelo	Lidocaine	17K23-B04-343250	1
Caelo	Lidocaine	17K23-B04-347473	1
Caelo	Lidocaine	17K23-B04-347475	1
Caelo	Lidocaine	17K23-B04-350189	1
Caelo	Lidocaine	17K23-B04-350543	1
Caelo	Lidocaine	17K23-B04-353247	1
Caelo	Lidocaine	17K23-B04-353427	1
Caelo	Lidocaine	18041812	1
Caelo	Lidocaine	1804404	1
Caelo	Lidocaine	1804410	1
Caelo	Lidocaine	1804413	2
Caelo	Lidocaine	18044402	5
Caelo	Lidocaine	18044404	9
Caelo	Lidocaine	18044405	8
Caelo	Lidocaine	18044408	7
Caelo	Lidocaine	18044410	12
Caelo	Lidocaine	18044412	2
Caelo	Lidocaine	18044413	17
Caelo	Lidocaine	18044414	1
Caelo	Lidocaine	18044415	6
Caelo	Lidocaine	180444404	1
Caelo	Lidocaine	190545001	15
Caelo	Lidocaine	19054503	15
Caelo	Lidocaine	19054503P-190909-3	1
Caelo	Lidocaine	19054505	8
Caelo	Lidocaine	19054506	18
Caelo	Lidocaine	19054507	2
Caelo	Lidocaine	192758001	5
Caelo	Lidocaine	192758002	1
Caelo	Lidocaine	192758003	1
Caelo	Lidocaine	192758004	8
Caelo	Lidocaine	192758005	13
Caelo	Lidocaine	19278005	1
Caelo	Lidocaine	1954503	1
Caelo	Lidocaine	19f27-b01-363506	2
Caelo	Lidocaine	19F27-B01-363506	1
Caelo	Lidocaine	20003343001	2
Caelo	Lidocaine	20003343002	5
Caelo	Lidocaine	20003343004	13
Caelo	Lidocaine	20003343006	3
Caelo	Lidocaine	20003343007	3
Caelo	Lidocaine	20003343008	11
Caelo	Lidocaine	20003343010	9
Caelo	Lidocaine	20003343011	4
Caelo	Lidocaine	20003343012	2
Caelo	Lidocaine	20003343014	3
Caelo	Lidocaine	20003343015	13
Caelo	Lidocaine	20003343016	5
Caelo	Lidocaine	2000334304	1
Caelo	Lidocaine	2000409002	1
Caelo	Lidocaine	20004099001	23
Caelo	Lidocaine	20004099002	2
Caelo	Lidocaine	2000409901	1
Caelo	Lidocaine	2003343008	1
Caelo	Lidocaine	200409900100	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lidocaine	2004099002	1
Caelo	Lidocaine	20C13-F04-369814	1
Caelo	Lidocaine	20H13-F04-3734909	1
Caelo	Lidocaine	22000398001	3
Caelo	Lidocaine	22000398003	2
Caelo	Lidocaine	22000398004	19
Caelo	Lidocaine	22000398010	2
Caelo	Lidocaine	22000398011	1
Caelo	Lidocaine	220600-01	1
Caelo	Lidocaine	5111201	1
Caelo	Lidocaine	8629595	1
Caelo	Lidocaine	9205916	2
Caelo	Lidocaine	9205919	1
Caelo	Lidocaine	LDB/733005	2
Caesar & Loretz noweda	Lidocaine	20003343015	2
Caesar & Loretz GmbH...	Lidocaine	20003343015	2
Caesar & Loretz GmbH...	Lidocaine	18044405	1
Caesar & Loretz GmbH /E	Lidocaine	18044413	1
Caesar & Loretz GmbH/ AHD	Lidocaine	20003343010	1
Caesar & Loretz GmbH...	Lidocaine	192758004	1
Caesar & Loretz GmbH...	Lidocaine	22000398010	1
Caesar & Loretz GmbH...	Lidocaine	20003343002	1
Caesar & Loretz GmbH/AHC	Lidocaine	20003343015	1
Caesar & Loretz GmbH...	Lidocaine	20004099001	1
Caesar & Loretz GmbH...	Lidocaine	19054505	1
Caesar & Loretz GmbH/Gehe	Lidocaine	20003343006	1
Caesar & Loretz GmbH/Gehe	Lidocaine	20003343011	2
Caesar & Loretz GmbH...	Lidocaine	192758005	1
Caesar & Loretz GmbH...	Lidocaine	20003343004	2
Caesar & Loretz GmbH...	Lidocaine	192758004	2
Caesar & Loretz GmbH...	Lidocaine	20003343002	3
Caesar & Loretz GmbH...	Lidocaine	18044410	1
Caesar & Loretz GmbH...	Lidocaine	192758005	1
Caesar & Loretz GmbH...	Lidocaine	20003343004	2
Caesar & Loretz GmbH...	Lidocaine	20003343008	1
Caesar & Loretz GmbH...	Lidocaine	20004099001	1
Caesar & Loretz GmbH...	Lidocaine	19054505	1
Caesar & Loretz GmbH	Lidocaine	12294412	1
Caesar & Loretz GmbH	Lidocaine	17K23_B04_355709	1
Caesar & Loretz GmbH	Lidocaine	18044408	1
Caesar & Loretz GmbH	Lidocaine	18044410	2
Caesar & Loretz GmbH	Lidocaine	18044414	2
Caesar & Loretz GmbH	Lidocaine	18044415	3
Caesar & Loretz GmbH	Lidocaine	190545001	5
Caesar & Loretz GmbH	Lidocaine	19054503	1
Caesar & Loretz GmbH	Lidocaine	19054505	1
Caesar & Loretz GmbH	Lidocaine	19054506	2
Caesar & Loretz GmbH	Lidocaine	19054507	1
Caesar & Loretz GmbH	Lidocaine	192758001	1
Caesar & Loretz GmbH	Lidocaine	192758003	1
Caesar & Loretz GmbH	Lidocaine	192758004	2
Caesar & Loretz GmbH	Lidocaine	20003343001	1
Caesar & Loretz GmbH	Lidocaine	20003343002	8
Caesar & Loretz GmbH	Lidocaine	20003343004	7
Caesar & Loretz GmbH	Lidocaine	20003343006	2
CAESAR & LORETZ GMBH	Lidocaine	20003343006	1
Caesar & Loretz GmbH	Lidocaine	20003343008	1
Caesar & Loretz GmbH	Lidocaine	20003343010	4
Caesar & Loretz GmbH	Lidocaine	20003343011	2
Caesar & Loretz GmbH	Lidocaine	20003343014	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Lidocaine	20003343015	5
Caesar & Loretz GmbH	Lidocaine	20003343016	2
Caesar & Loretz GmbH	Lidocaine	20004099001	9
Caesar & Loretz GmbH	Lidocaine	22000398004	4
Caesar & Loretz GmbH	Lidocaine	22C15-B17-216739	1
Caesar & Loretz GmbHGehe	Lidocaine	22000398016	1
Caesar & Loretz Hilden	Lidocaine	19054506	1
Caesar&Loretz GmbH	Lidocaine	16289502	1
Caesar&Loretz,Phönix...	Lidocaine	15332314	1
Cealo / Anzag	Lidocaine	211217(20003343008)	1
Cealo	Lidocaine	17348503	1
Ebert-Jacobi	Lidocaine	16289504	1
Eur Rho Gehe	Lidocaine	1908005-92	1
EuRho, Noweda	Lidocaine	2101035-03	1
Euro OTC	Lidocaine	10129901	1
Euro OTC	Lidocaine	1310023-02	3
Euro OTC	Lidocaine	1603027-01	2
Euro OTC	Lidocaine	1603027-02	1
Euro OTC	Lidocaine	1612021-01	5
Euro OTC	Lidocaine	161202102	2
Euro OTC	Lidocaine	1612021-02	6
Euro OTC	Lidocaine	1612021-03	4
Euro OTC	Lidocaine	1612021-04	6
Euro OTC	Lidocaine	17348503	1
Euro OTC	Lidocaine	17K23B04345215	1
Euro OTC	Lidocaine	17K23-B04-347473	1
Euro OTC	Lidocaine	190200301	1
Euro OTC	Lidocaine	1902003-01	4
Euro OTC	Lidocaine	1905004-01	1
Euro OTC	Lidocaine	190800501	1
Euro OTC	Lidocaine	1908005-01	18
Euro OTC	Lidocaine	1908005-02	9
Euro OTC	Lidocaine	1911005-01	3
Euro OTC	Lidocaine	2006013-01	7
Euro OTC	Lidocaine	2101035-01	8
Euro OTC	Lidocaine	210103502	1
Euro OTC	Lidocaine	2101035-02	7
Euro OTC	Lidocaine	2101035-03	5
Euro OTC	Lidocaine	2206002-01	1
Euro OTC	Lidocaine	2206002-02	3
Euro OTC	Lidocaine	LD/119024	1
Euro OTC	Lidocaine	LDB/116106	1
Euro OTC	Lidocaine	LDB/120025	1
Fagro/Gehe	Lidocaine	15a15b01304284	1
Fagron	Lidocaine		2
Fagron	Lidocaine	1014I-07006	1
Fagron	Lidocaine	1113M-03584	1
Fagron	Lidocaine	1116E-07006	1
Fagron	Lidocaine	118J23-B02-359239	1
Fagron	Lidocaine	11C09-N07	2
Fagron	Lidocaine	11D28-N12	1
Fagron	Lidocaine	11K17-N03	1
Fagron	Lidocaine	12/21-N06	3
Fagron	Lidocaine	12C08-N11	2
Fagron	Lidocaine	12E30-N10	8
Fagron	Lidocaine	12h16_n05	1
Fagron	Lidocaine	12h16-N05	1
Fagron	Lidocaine	12H16-n05	1
Fagron	Lidocaine	12H16-N05	5
Fagron	Lidocaine	12I21N06	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Lidocaine	12I21-N06	3
Fagron	Lidocaine	12K13-N01	1
Fagron	Lidocaine	1330-B02-287641	1
Fagron	Lidocaine	13B27-N04	8
Fagron	Lidocaine	13E28-B40-289433	1
Fagron	Lidocaine	13H05-N05	10
Fagron	Lidocaine	13H05-N050171/245	1
Fagron	Lidocaine	13J30-B02	6
Fagron	Lidocaine	13J30-b02-287639	1
Fagron	Lidocaine	13J30-B02-287640	1
Fagron	Lidocaine	13J30-B02-287641	6
Fagron	Lidocaine	13j30B02292219	1
Fagron	Lidocaine	13J30-B02-292219	2
Fagron	Lidocaine	13J30-B02-292220	2
Fagron	Lidocaine	13J30-B02-292221	5
Fagron	Lidocaine	14E13-B05	2
Fagron	Lidocaine	14E13-B05-295549	4
Fagron	Lidocaine	14E13-B05-295550	2
Fagron	Lidocaine	14E13-B05-295552	3
Fagron	Lidocaine	15332305	1
Fagron	Lidocaine	15A15-B01	1
Fagron	Lidocaine	15A15-B01-304282	5
Fagron	Lidocaine	15A15-B01-304283	2
Fagron	Lidocaine	15A15B01304284	1
Fagron	Lidocaine	15A15-B01-304284	10
Fagron	Lidocaine	15D23-B08	1
Fagron	Lidocaine	15D23-B08_309882	1
Fagron	Lidocaine	15D23-B08_312058	1
Fagron	Lidocaine	15d23-b08-309882	1
Fagron	Lidocaine	15D23-B08-309882	1
Fagron	Lidocaine	15D23-B08-31058	1
Fagron	Lidocaine	15D23B08311708	1
Fagron	Lidocaine	15D23-B08-311708	1
Fagron	Lidocaine	15d23-b08-312058	2
Fagron	Lidocaine	15D23-B08-312058	11
Fagron	Lidocaine	15h27-b05-318310	1
Fagron	Lidocaine	15H27-B07	1
Fagron	Lidocaine	15H27-B07-315483	2
Fagron	Lidocaine	15H27-B07-316784	2
Fagron	Lidocaine	15H27-B07-318310	5
Fagron	Lidocaine	1612021-01	1
Fagron	Lidocaine	16289508	1
Fagron	Lidocaine	16A28B06320059	1
Fagron	Lidocaine	16A28-B06-320059	2
Fagron	Lidocaine	16A28-B06320079	1
Fagron	Lidocaine	16A28-B06-320079	1
Fagron	Lidocaine	16F21	2
Fagron	Lidocaine	16F21-B06	7
Fagron	Lidocaine	16F21-B06-323669	5
Fagron	Lidocaine	16F21-B06-323670	18
Fagron	Lidocaine	16F21B06325934	1
Fagron	Lidocaine	16F21-B06-325934	3
Fagron	Lidocaine	16F21-B06-327232	3
Fagron	Lidocaine	16F21-B06-328421	8
Fagron	Lidocaine	16F21-B06-328421	1
Fagron	Lidocaine	16F21-B06-329589	1
Fagron	Lidocaine	16F21B06332251	1
Fagron	Lidocaine	16F21-B06-332253	6
Fagron	Lidocaine	16F21-B06-332253	1
Fagron	Lidocaine	16F21B06333787	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Lidocaine	16F21-B06-333787	1
Fagron	Lidocaine	16F21-B06-333788	1
Fagron	Lidocaine	16f21-b06-335659	1
Fagron	Lidocaine	16F21-B06-335659	1
Fagron	Lidocaine	17G03-B08	5
Fagron	Lidocaine	17G03-B08-337576	2
Fagron	Lidocaine	17G03-B08-338284	1
Fagron	Lidocaine	17g03-b08-338286	1
Fagron	Lidocaine	17G03-B08-338286	6
Fagron	Lidocaine	17G03-B08-339445	2
Fagron	Lidocaine	17G03-B08-341306	5
Fagron	Lidocaine	17G03-B08-341308	5
Fagron	Lidocaine	17G03-B08-343251	4
Fagron	Lidocaine	17G23-B04-350541	1
Fagron	Lidocaine	17K23-B04	16
Fagron	Lidocaine	17K23-B04-343250	6
Fagron	Lidocaine	17K23-B04-345215	10
Fagron	Lidocaine	17K23-B04-345948	3
Fagron	Lidocaine	17K23B04347473	2
Fagron	Lidocaine	17K23-B04-347473	7
Fagron	Lidocaine	17K23B04347474	1
Fagron	Lidocaine	17K23-B04-347474	4
Fagron	Lidocaine	17k23-b04-347475	1
Fagron	Lidocaine	17K23-B04-347475	9
Fagron	Lidocaine	17k23-b04-349366	1
Fagron	Lidocaine	17K23B04350189	1
Fagron	Lidocaine	17K23-B04-350189	5
Fagron	Lidocaine	17K23-B04-350541	8
Fagron	Lidocaine	17K23-B04-350542	2
Fagron	Lidocaine	17K23-B04-350543	13
Fagron	Lidocaine	17K23-B04-353247	7
Fagron	Lidocaine	17k23-b04-353427	1
Fagron	Lidocaine	17K23-B04-353427	7
Fagron	Lidocaine	17K23-B04-3534274	1
Fagron	Lidocaine	17K23B04353428	1
Fagron	Lidocaine	17K23-B04-353428	7
Fagron	Lidocaine	17K23-B04-355709	13
Fagron	Lidocaine	17K23-B04-355750	1
Fagron	Lidocaine	18/23-B02-359237	1
Fagron	Lidocaine	18/23-B02-359239	1
Fagron	Lidocaine	1823-B02-356573	1
Fagron	Lidocaine	18J23-B02	8
Fagron	Lidocaine	18J23-B02_359237	1
Fagron	Lidocaine	18J23-B02-3557018	1
Fagron	Lidocaine	18J23-B02-355708	4
Fagron	Lidocaine	18J23-B02356573	1
Fagron	Lidocaine	18J-23-B02-356573	1
Fagron	Lidocaine	18J23-B02-35673	1
Fagron	Lidocaine	18j23-B02-359237	1
Fagron	Lidocaine	18J23-B02-359237	5
Fagron	Lidocaine	18J23-B02-359238	3
Fagron	Lidocaine	18J23B02359239	1
Fagron	Lidocaine	18J23-B02-359239	22
Fagron	Lidocaine	18j23bo2359239	1
Fagron	Lidocaine	190545001	1
Fagron	Lidocaine	190981109	1
Fagron	Lidocaine	19F27-B01	18
Fagron	Lidocaine	19F27-B01363500	1
Fagron	Lidocaine	19F27-B01-363500	7
Fagron	Lidocaine	19F27-B01-3635005	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Lidocaine	19F27-B01-3635006	1
Fagron	Lidocaine	19f27-B01-363501	1
Fagron	Lidocaine	19F27-B01-363501	21
Fagron	Lidocaine	19F27-B01-363502	12
Fagron	Lidocaine	19f27b01363504	1
Fagron	Lidocaine	19F27-b01-363504	1
Fagron	Lidocaine	19F27-B01363504	1
Fagron	Lidocaine	19F27-B01-363504	10
Fagron	Lidocaine	19F27-B01-363505	8
Fagron	Lidocaine	19F27-B01-363506	15
Fagron	Lidocaine	19F27-B01-363511	1
Fagron	Lidocaine	19F27-Bo1-363504	2
Fagron	Lidocaine	19F27-BO1-363506	2
Fagron	Lidocaine	20C13-F04	4
Fagron	Lidocaine	20C13-F04-3698105	1
Fagron	Lidocaine	20C13-F04-3698106	1
Fagron	Lidocaine	20C13-F04-369814	4
Fagron	Lidocaine	20c13-F04-369815	1
Fagron	Lidocaine	20C13-F04-369815	9
Fagron	Lidocaine	20C13-F04-369816	13
Fagron	Lidocaine	20H13-F03	4
Fagron	Lidocaine	20H13-F03-373500	1
Fagron	Lidocaine	20H13-F03-373501	1
Fagron	Lidocaine	20H13-F04	4
Fagron	Lidocaine	20H13-F04-3734907	1
Fagron	Lidocaine	20H13-f04-373497	1
Fagron	Lidocaine	20H13-F04-373497	16
Fagron	Lidocaine	20H13-F04-373499	3
Fagron	Lidocaine	20H13-F04-373501	1
Fagron	Lidocaine	20h13-f04-73497	1
Fagron	Lidocaine	20H13-FO-373497	1
Fagron	Lidocaine	20H13FO4-373497	1
Fagron	Lidocaine	20ht3-f04-373497	1
Fagron	Lidocaine	20L11-F01	4
Fagron	Lidocaine	20L11-F01_376357	1
Fagron	Lidocaine	20L11-F01-376356	2
Fagron	Lidocaine	20l11-f01-376357	1
Fagron	Lidocaine	20L11-f01-376357	1
Fagron	Lidocaine	20L11-F01-376357	9
Fagron	Lidocaine	20M13-F04-373497	1
Fagron	Lidocaine	214U-03584	1
Fagron	Lidocaine	21B10-B07	1
Fagron	Lidocaine	21B10-B07-213330	3
Fagron	Lidocaine	21B10-B07-213578	1
Fagron	Lidocaine	21f08b14216888	1
Fagron	Lidocaine	22C115-B17-216739	1
Fagron	Lidocaine	22C15-817-216739	1
Fagron	Lidocaine	22C15-B17	2
Fagron	Lidocaine	22C15-B17_216737	1
Fagron	Lidocaine	22C15-B17-216737	9
Fagron	Lidocaine	22C15-B17-216738	10
Fagron	Lidocaine	22c15b17216739	1
Fagron	Lidocaine	22c15-b17-216739	1
Fagron	Lidocaine	22C15-B17-216739	20
Fagron	Lidocaine	22C15-B17-221066	1
Fagron	Lidocaine	22C15-B17-225236	1
Fagron	Lidocaine	22C15-B17-225237	1
Fagron	Lidocaine	20L11-FO1-376357	1
Fagron	Lidocaine	369816	1
Fagron	Lidocaine	5122014A	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Lidocaine	515M-07006	1
Fagron	Lidocaine	5742	1
Fagron	Lidocaine	6J23-No2	1
Fagron	Lidocaine	700412-0002	1
Fagron	Lidocaine	700412-0004	1
Fagron	Lidocaine	700412-0006	1
Fagron	Lidocaine	71-18	1
Fagron	Lidocaine	8J23-B02-3592391	1
Fagron	Lidocaine	B01-3635001	1
Fagron	Lidocaine	B01-3635002	1
Fagron	Lidocaine	B01-3635004	3
Fagron	Lidocaine	B01-3635006	2
Fagron	Lidocaine	B07-318310	1
Fagron	Lidocaine	F01-3763507	1
Fagron	Lidocaine	F03-3735001	1
Fagron	Lidocaine	F0-37349	1
Fagron	Lidocaine	F04-3698104	1
Fagron	Lidocaine	F04-3698105	2
Fagron	Lidocaine	F04-3698106	3
Fagron	Lidocaine	F04-3734907	1
Fagron	Lidocaine	F04-3734909	2
Fagron	Lidocaine	LDB/116049	2
Fagron	Lidocaine	LDB/117049	1
Fagron	Lidocaine	LDB/117093	4
Fagron	Lidocaine	LDB/118066	2
Fagron	Lidocaine	LDB/119043	5
Fagron	Lidocaine	LDB/119043x3	1
Fagron	Lidocaine	ldb/120006	1
Fagron	Lidocaine	LDB/120006	3
Fagron	Lidocaine	LDB/120018	2
Fagron	Lidocaine	LDB/722005	3
Fargon/ Sanacorp Lübeck	Lidocaine	18J23-B02-359237	1
Fargon/AHD	Lidocaine	17K23-B04-353428	1
Fargon/AHD	Lidocaine	18J23-B02-359238	1
Fargon/Fönix	Lidocaine	20C13-F04-369814	1
Fargon/Noweda	Lidocaine	17K23-B04-350543	1
Fargon/Noweda	Lidocaine	19F27-B01	1
Fargon/Phoenix	Lidocaine	13H05-N05	3
Fargon	Lidocaine	12E30-N10	1
Fargron	Lidocaine	14E13-B05-295552	1
Faron/Alliance	Lidocaine	16F21-B06-323670	2
Fragon/ Gehe	Lidocaine	19F27-B01-363502	1
Gatt-Koller	Lidocaine	1900471	1
GEHE 02.12.2014	Lidocaine	13J30-B02-292220	1
Gehe am 22.01.2014	Lidocaine	13H05-N05	2
Gehe Kassel	Lidocaine	14E13-B05-295550	1
Gehe	Lidocaine	12H16-N05	1
Gehe	Lidocaine	13B27-N04	1
Gehe	Lidocaine	14E13-B05-295552	1
GEHE	Lidocaine	16289503	1
Gehe	Lidocaine	16F21-B06-323670	1
GEHE	Lidocaine	16F21-B06-328421	1
Gehe	Lidocaine	17G03-B08-338286	2
Gehe	Lidocaine	17K23-B04-355709	1
GEHE	Lidocaine	18044405	1
Gehe	Lidocaine	18J23-B02-359239	1
Gehe	Lidocaine	19054505	2
Gehe	Lidocaine	192758005	2
Gehe	Lidocaine	20C13F04369816	1
Gehe	Lidocaine	22000398011	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Lidocaine	22000398016	1
Gehe	Lidocaine	22C15-B17-216739	1
Gehe	Lidocaine	23D25-B10-230220	1
Gehe	Lidocaine	23D25-B10-230226	1
GEHE	Lidocaine	23D25-B10-234510	1
Gehe	Lidocaine	23H23-B01-234506	1
Geilenkirchen	Lidocaine	17G03-B08-341306	1
Geilenkirchen	Lidocaine	LDB/117093	1
Geilenkirchen	Lidocaine	LDB/118066	1
GUMO	Lidocaine	19F27-B01-3635006	2
Gutenberg-Apotheke	Lidocaine	13J30-B02	1
Hedinger/Gehe	Lidocaine	17K23-B04-343250	1
Henry Lamotte Oils GmbH	Lidocaine		1
Jenne	Lidocaine	20003343015	1
Jenne	Lidocaine	2101035-02	1
Kehr	Lidocaine	16F21-B06-328421	1
Kehr	Lidocaine	16F21-B06-332251	1
Kehr	Lidocaine	17G03-B08-338284	1
Kehr	Lidocaine	22000398013	1
Kehr	Lidocaine	22C15-B17-216739	1
LaVita	Lidocaine	15H27-B07-318310	1
Moehs BCN S.L. / Noweda	Lidocaine	15332305	1
Nachprüfung von Juni 2018	Lidocaine	12C08-N11	1
Noweda	Lidocaine	10129901	1
Noweda	Lidocaine	12H16-N05	3
Noweda	Lidocaine	12H16-No5	1
Noweda	Lidocaine	16F21-B06	1
Noweda	Lidocaine	17K23-B04-347473	1
Noweda	Lidocaine	17K23-B04-350542	1
Noweda	Lidocaine	18044402	1
Noweda	Lidocaine	18J23-B02-355708	3
Noweda	Lidocaine	19054503	1
Noweda	Lidocaine	192758005	1
Noweda	Lidocaine	2003343016	1
Noweda	Lidocaine	220003908013	1
Noweda	Lidocaine	22000398013	1
Pharmachem	Lidocaine	17K23-B04-350541	1
PHOENIX 22.08.2014	Lidocaine		2
PHOENIX 22.08.2014	Lidocaine	13J30-B02-287640	1
Phoenix	Lidocaine	15332305	1
phoenix	Lidocaine	17348503	1
Phoenix	Lidocaine	17K23-B04-350543	1
Phoenix	Lidocaine	17K23-B05-345948	1
Phoenix	Lidocaine	18J23-B02-359238	1
Phoenix	Lidocaine	1905004-01	1
Phoenix	Lidocaine	19054504	1
Phoenix	Lidocaine	19f27-b01	1
Phoenix	Lidocaine	20003343004	1
Phoenix	Lidocaine	20004099001	1
Phoenix	Lidocaine	20c13-f04-369815	1
Phoenix	Lidocaine	20h13-f03-373501	1
Phoenix	Lidocaine	20H13-F04-373497	1
Phönix Gotha	Lidocaine	15A15-B01-304284	1
Phönix	Lidocaine	13352405	1
Phönix	Lidocaine	13B27-N04	1
Phönix	Lidocaine	17K23-B04-343250	1
Phönix	Lidocaine	17K23-B04-345215	1
Phönix	Lidocaine	17K23-B04-347475	1
Phönix	Lidocaine	19F27-B01-363505	1
Phönix	Lidocaine	2006013-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Lidocaine	200860209	1
PHönix	Lidocaine	20h13-f04-373499	1
Rondell Apotheke	Lidocaine	15332304	1
Sanacorp	Lidocaine	12H16-N05	1
Sanacorp	Lidocaine	12I21-N06	1
Sanacorp	Lidocaine	1603027-02	1
Sanacorp	Lidocaine	17183109	1
Sanacorp	Lidocaine	17K23-B04-350542	1
Sanacorp	Lidocaine	22000398011	2
Sanacorp	Lidocaine	22000398013	1
Sanacorp	Lidocaine	226002-01	1
Sanacorp	Lidocaine	22C15-B17-225236	1
Sanacorp	Lidocaine	22C15-B17-225237	3
Sanacorp	Lidocaine	23D25-B10-230221	1
Spangropharm	Lidocaine	18044410	1
Swati Pentose/ Link ...	Lidocaine	B2185	1
Swati Spentose / Gehe	Lidocaine	18J23-B02-359237	1
Swati Spentose / Gehe	Lidocaine	19F27-B01-363500	1
Swati Spentose / Gehe	Lidocaine	B01-3635001	1
SWATI SPENTOSE PRIVATE	Lidocaine	2101035-03	2
Swati Spentose Pvt L...	Lidocaine	B2185	1
Swati Spentose Pvt.L...	Lidocaine	21B10-B07213330	1
Swati Spentose Pvt.L...	Lidocaine	21B10-B07-213330	1
SWATI/Noweda	Lidocaine	LDB/119024	1
Swato Spentosen/Phoenix	Lidocaine	F04-3698105	1

- 234 339 spectra from 1515 *Apo-Ident* customers from a total of 48 845 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Lidocaine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lidocaine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	600	0	201 484
Type C	0	1718	10	234 339

The substance/substance group *Lidocaine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0000 %)
Type C	100.0000 % (> 99.9007 %)	99.4213 % (> 99.2477 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20942	20942	0.00	165.68
21640	24031	12.94	164.79
21673	24031	29.42	166.65
22984	22984	0.00	164.26
23019	22984	6.32	164.00
24031	24031	0.00	165.86
24928	24928	0.00	164.61
25533	25533	0.00	163.46
26654	26654	0.00	163.44

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Lidocaine hydrochloride monohydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20093-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lidocaine hydrochloride monohydrate; Lidocaini hydrochloridum monohydricum

Special notes

When selecting the *Lidocaine hydrochloride monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Lidocaine hydrochloride monohydrate	7	14	478

Second-stage model

For differentiation of the substance/substance group *Lidocaine hydrochloride monohydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Lidocaine hydrochloride monohydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	104.85	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Lidocaine hydrochloride monohydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Lidocaine hydrochloride monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Lidocaine hydrochloride m…	12135511	20882	40	AR-15-FG-008867-01
Caelo	Lidocaine hydrochloride m…	172923	23807	40	20171122*
Euro OTC	Lidocaine hydrochloride m…	1403025-02	21613	60	20140516
Euro OTC	Lidocaine hydrochloride m…	1411010	21770	60	20150126*
Euro OTC	Lidocaine hydrochloride m…	1907012	24776	40	20190801*
Euro OTC	Lidocaine hydrochloride m…	2201026	26028	40	20220321*
Fagron	Lidocaine hydrochloride m…	20C18-B02-196984	25446	40	20200324

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 320 spectra of 7 reference samples from the substance/substance group *Lidocaine hydrochloride monohydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 642 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 620 spectra of 17 reference samples from the substance/substance group *Lidocaine hydrochloride monohydrate*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Lidocaine hydrochloride m…	162222	22771	40
Caelo	Lidocaine hydrochloride m…	152995	22772	40
Caelo	Lidocaine hydrochloride m…	172048	23687	40
Caelo	Lidocaine hydrochloride m…	20001694	25626	40
Caelo	Lidocaine hydrochloride m…	21002505	25852	50
Caelo	Lidocaine hydrochloride m…	22003202	26491	40
Caelo	Lidocaine hydrochloride m…	23002422	26945	40
Euro OTC	Lidocaine hydrochloride m…	1606024	22702	40
Euro OTC	Lidocaine hydrochloride m…	1612015	22980	40
Euro OTC	Lidocaine hydrochloride m…	1808031	24326	40
Euro OTC	Lidocaine hydrochloride m…	2101034	25572	40
Euro OTC	Lidocaine hydrochloride m…	2211019	26523	40
Euro OTC	Lidocaine hydrochloride m…	2405011	27339	40
Fagron	Lidocaine hydrochloride m…	22C15-B16-218866	26135	40
Caelo	Lidocaine hydrochloride m…	22003202	26491SI	20
Euro OTC	Lidocaine hydrochloride m…	2201026	26028SI†	10
Fagron	Lidocaine hydrochloride m…	22C15-B16-218866	26135SI	20

- 201 464 spectra from a total of 4030 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3659 spectra from 1120 *Apo-Ident* customers from 497 batches from the substance/substance group *Lidocaine hydrochloride monohydrate*.
- Among them are spectra of independent samples from 474 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Lidocaine hydrochloride m...		1
	Lidocaine hydrochloride m...	21002505006	2
	Lidocaine hydrochloride m...	21002505007	2
	Lidocaine hydrochloride m...	21002505012	2
	Lidocaine hydrochloride m...	2101034-03	2
	Lidocaine hydrochloride m...	220032004	1
	Lidocaine hydrochloride m...	22003202002	11
	Lidocaine hydrochloride m...	22003202003	10
	Lidocaine hydrochloride m...	22003202004	1
	Lidocaine hydrochloride m...	22003202006	5
	Lidocaine hydrochloride m...	22003202007	3
	Lidocaine hydrochloride m...	2201026-01	4
	Lidocaine hydrochloride m...	2201026-02	12
	Lidocaine hydrochloride m...	22110019-003	1
	Lidocaine hydrochloride m...	22110119-01	1
	Lidocaine hydrochloride m...	221101901	1
	Lidocaine hydrochloride m...	2211019-01	70
	Lidocaine hydrochloride m...	2211019-02	8
	Lidocaine hydrochloride m...	2211019-03	4
	Lidocaine hydrochloride m...	22C15-B16-218866	1
	Lidocaine hydrochloride m...	22C15-B16-220953	1
	Lidocaine hydrochloride m...	23003452004	4
	Lidocaine hydrochloride m...	23D25-B11-230225	1
	Lidocaine hydrochloride m...	2405011-01	1
	Lidocaine hydrochloride m...	245011-02	1
	Lidocaine hydrochloride m...	LDH/121043	2
01.07.14	Lidocaine hydrochloride m...	13343004	1
08597954	Lidocaine hydrochloride m...	1907012-01	1
A.H.D.	Lidocaine hydrochloride m...	1202035-02	1
ACM	Lidocaine hydrochloride m...	KNC0625J17	1
ACM	Lidocaine hydrochloride m...	KNC1247J15	1
AEP	Lidocaine hydrochloride m...	22003202003	1
AHC	Lidocaine hydrochloride m...	2211019-02	1
AHD	Lidocaine hydrochloride m...	1612015-02	1
AHD	Lidocaine hydrochloride m...	17292308	2
AHD	Lidocaine hydrochloride m...	17292311	1
AHD	Lidocaine hydrochloride m...	17292313	1
AHD	Lidocaine hydrochloride m...	18179904	1
AHD	Lidocaine hydrochloride m...	18179910	1
AHD	Lidocaine hydrochloride m...	22003202003	1
AHD	Lidocaine hydrochloride m...	2211019-01	2
AHD	Lidocaine hydrochloride m...	23003452004	1
ALH/EuRho	Lidocaine hydrochloride m...	1612015-01	1
ALH	Lidocaine hydrochloride m...	1606024-01	1
Alliance Healt	Lidocaine hydrochloride m...	LDH/722031	1
Alliance health	Lidocaine hydrochloride m...	14B12-B03-292214	1
Alliance	Lidocaine hydrochloride m...	2101034-03	1
Alliance	Lidocaine hydrochloride m...	2211019-01	6
Allianz	Lidocaine hydrochloride m...	17292308	1
Alte Apotheke	Lidocaine hydrochloride m...	1606024-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Anzag	Lidocaine hydrochloride m...	1202035-03	1
Anzag	Lidocaine hydrochloride m...	1403025-01	1
Anzag	Lidocaine hydrochloride m...	1411010-01	1
Anzag	Lidocaine hydrochloride m...	14B12-B03-292214	1
Anzag	Lidocaine hydrochloride m...	17204804	2
Anzag	Lidocaine hydrochloride m...	1907012-02	1
Anzag	Lidocaine hydrochloride m...	2101034-03	2
Anzag	Lidocaine hydrochloride m...	23003452002	1
Apoident /Sanacorp	Lidocaine hydrochloride m...	2101034-01	2
Apo-Ident, Phönix, 7...	Lidocaine hydrochloride m...	1612015-01	1
apoident/AHD	Lidocaine hydrochloride m...	1808031-03	1
Apo-ident	Lidocaine hydrochloride m...	2101034-02	1
Apo-ident	Lidocaine hydrochloride m...	2101034-03	1
Apo-ident	Lidocaine hydrochloride m...	2201026-01	1
Audor Pharma	Lidocaine hydrochloride m...	2101034-01	1
Bombastus	Lidocaine hydrochloride m...	15215301	1
Bombastus	Lidocaine hydrochloride m...	1606024-01	6
Bombastus	Lidocaine hydrochloride m...	1612015-02	1
Bombastus	Lidocaine hydrochloride m...	180831-01	1
Caelo	Lidocaine hydrochloride m...		1
Caelo	Lidocaine hydrochloride m...	1017Q-01775	1
Caelo	Lidocaine hydrochloride m...	10320703	1
Caelo	Lidocaine hydrochloride m...	10320704	1
Caelo	Lidocaine hydrochloride m...	10320707	2
Caelo	Lidocaine hydrochloride m...	10320717	1
Caelo	Lidocaine hydrochloride m...	10320719	1
Caelo	Lidocaine hydrochloride m...	11091203	1
Caelo	Lidocaine hydrochloride m...	11302902	2
Caelo	Lidocaine hydrochloride m...	11302904	1
Caelo	Lidocaine hydrochloride m...	11302905	1
Caelo	Lidocaine hydrochloride m...	11302906	3
Caelo	Lidocaine hydrochloride m...	116037	1
Caelo	Lidocaine hydrochloride m...	1202035	1
Caelo	Lidocaine hydrochloride m...	120203501	1
Caelo	Lidocaine hydrochloride m...	1202035-02	5
Caelo	Lidocaine hydrochloride m...	1202035-03	1
Caelo	Lidocaine hydrochloride m...	12021503	1
Caelo	Lidocaine hydrochloride m...	12135503	2
Caelo	Lidocaine hydrochloride m...	12135504	3
Caelo	Lidocaine hydrochloride m...	12135508	5
Caelo	Lidocaine hydrochloride m...	12135509	4
Caelo	Lidocaine hydrochloride m...	12135511	2
Caelo	Lidocaine hydrochloride m...	12176101	8
Caelo	Lidocaine hydrochloride m...	12176102	8
Caelo	Lidocaine hydrochloride m...	12176103	8
Caelo	Lidocaine hydrochloride m...	12176109	2
Caelo	Lidocaine hydrochloride m...	1230817/160602402	1
Caelo	Lidocaine hydrochloride m...	12B23-B03-352117	1
Caelo	Lidocaine hydrochloride m...	13(1808031-01)	1
Caelo	Lidocaine hydrochloride m...	13118802	2
Caelo	Lidocaine hydrochloride m...	13118803	5
Caelo	Lidocaine hydrochloride m...	13118807	6
Caelo	Lidocaine hydrochloride m...	13118808	4
Caelo	Lidocaine hydrochloride m...	13118811	2
Caelo	Lidocaine hydrochloride m...	13118812	3
Caelo	Lidocaine hydrochloride m...	1317I-01775	1
Caelo	Lidocaine hydrochloride m...	13343001	2
Caelo	Lidocaine hydrochloride m...	13343002	3
Caelo	Lidocaine hydrochloride m...	13343003	5
Caelo	Lidocaine hydrochloride m...	13343004	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lidocaine hydrochloride m…	13343007	12
Caelo	Lidocaine hydrochloride m…	13343008	5
Caelo	Lidocaine hydrochloride m…	13343011	3
Caelo	Lidocaine hydrochloride m…	13343012	17
Caelo	Lidocaine hydrochloride m…	13343014	5
Caelo	Lidocaine hydrochloride m…	13343015	2
Caelo	Lidocaine hydrochloride m…	13343016	2
Caelo	Lidocaine hydrochloride m…	13343017	5
Caelo	Lidocaine hydrochloride m…	13343019	4
Caelo	Lidocaine hydrochloride m…	1403025-02	2
Caelo	Lidocaine hydrochloride m…	1411010-01	2
Caelo	Lidocaine hydrochloride m…	1411010-02	1
Caelo	Lidocaine hydrochloride m…	14110101	1
Caelo	Lidocaine hydrochloride m…	14254001	3
Caelo	Lidocaine hydrochloride m…	14J20-B05-303131	1
Caelo	Lidocaine hydrochloride m…	14J20-B05-303133	1
Caelo	Lidocaine hydrochloride m…	15/17-B01-316805	1
Caelo	Lidocaine hydrochloride m…	1505023-01	6
Caelo	Lidocaine hydrochloride m…	1505023-02	2
Caelo	Lidocaine hydrochloride m…	1505023-03	2
Caelo	Lidocaine hydrochloride m…	1515I-01775	1
Caelo	Lidocaine hydrochloride m…	1517-B01-315828	1
Caelo	Lidocaine hydrochloride m…	1521304	1
Caelo	Lidocaine hydrochloride m…	15215201	3
Caelo	Lidocaine hydrochloride m…	15215301	8
Caelo	Lidocaine hydrochloride m…	15215302	2
Caelo	Lidocaine hydrochloride m…	15215303	2
Caelo	Lidocaine hydrochloride m…	15215304	3
Caelo	Lidocaine hydrochloride m…	15215308	3
Caelo	Lidocaine hydrochloride m…	15215309	3
Caelo	Lidocaine hydrochloride m…	15215310	10
Caelo	Lidocaine hydrochloride m…	15215311	6
Caelo	Lidocaine hydrochloride m…	15215312	7
Caelo	Lidocaine hydrochloride m…	152951602714117	1
Caelo	Lidocaine hydrochloride m…	1529906	1
Caelo	Lidocaine hydrochloride m…	15299502	1
Caelo	Lidocaine hydrochloride m…	15299503	11
Caelo	Lidocaine hydrochloride m…	15299506	6
Caelo	Lidocaine hydrochloride m…	15299509	3
Caelo	Lidocaine hydrochloride m…	15299513	9
Caelo	Lidocaine hydrochloride m…	15299514	10
Caelo	Lidocaine hydrochloride m…	15299516	12
Caelo	Lidocaine hydrochloride m…	15299816	1
Caelo	Lidocaine hydrochloride m…	15117-B01	1
Caelo	Lidocaine hydrochloride m…	1603027-01	1
Caelo	Lidocaine hydrochloride m…	1606024	1
Caelo	Lidocaine hydrochloride m…	160602401	1
Caelo	Lidocaine hydrochloride m…	1606024-01	20
Caelo	Lidocaine hydrochloride m…	1606024-02	5
Caelo	Lidocaine hydrochloride m…	160602403	1
Caelo	Lidocaine hydrochloride m…	1606024-03	3
Caelo	Lidocaine hydrochloride m…	160719LC	1
Caelo	Lidocaine hydrochloride m…	16083001	1
Caelo	Lidocaine hydrochloride m…	16101407	1
Caelo	Lidocaine hydrochloride m…	1612015	1
Caelo	Lidocaine hydrochloride m…	1612015_02	1
Caelo	Lidocaine hydrochloride m…	1612015-01	4
Caelo	Lidocaine hydrochloride m…	1612015-02	8
Caelo	Lidocaine hydrochloride m…	1612015-03	4
Caelo	Lidocaine hydrochloride m…	1612015-04	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lidocaine hydrochloride m...	1612015-05	1
Caelo	Lidocaine hydrochloride m...	16120515-02	1
Caelo	Lidocaine hydrochloride m...	16222202	2
Caelo	Lidocaine hydrochloride m...	16222203	8
Caelo	Lidocaine hydrochloride m...	16222206	2
Caelo	Lidocaine hydrochloride m...	16222207	8
Caelo	Lidocaine hydrochloride m...	16222208	6
Caelo	Lidocaine hydrochloride m...	16222214	13
Caelo	Lidocaine hydrochloride m...	16222215	1
Caelo	Lidocaine hydrochloride m...	168020-0003	1
Caelo	Lidocaine hydrochloride m...	16C09-B03-322144	1
Caelo	Lidocaine hydrochloride m...	17204803	14
Caelo	Lidocaine hydrochloride m...	17204804	32
Caelo	Lidocaine hydrochloride m...	17204810	3
Caelo	Lidocaine hydrochloride m...	17292301	2
Caelo	Lidocaine hydrochloride m...	17292302	6
Caelo	Lidocaine hydrochloride m...	17292304	27
Caelo	Lidocaine hydrochloride m...	17292304907012-02	1
Caelo	Lidocaine hydrochloride m...	17292305	1
Caelo	Lidocaine hydrochloride m...	17292307	5
Caelo	Lidocaine hydrochloride m...	17292308	9
Caelo	Lidocaine hydrochloride m...	17292310	1
Caelo	Lidocaine hydrochloride m...	17292311	9
Caelo	Lidocaine hydrochloride m...	17292313	8
Caelo	Lidocaine hydrochloride m...	17292316	3
Caelo	Lidocaine hydrochloride m...	1729308	1
Caelo	Lidocaine hydrochloride m...	1729311	1
Caelo	Lidocaine hydrochloride m...	1729313	1
Caelo	Lidocaine hydrochloride m...	1792304	1
Caelo	Lidocaine hydrochloride m...	1792313	1
Caelo	Lidocaine hydrochloride m...	17A16-B07	1
Caelo	Lidocaine hydrochloride m...	18041501	1
Caelo	Lidocaine hydrochloride m...	1808031	1
Caelo	Lidocaine hydrochloride m...	1808031-01	12
Caelo	Lidocaine hydrochloride m...	1808031-02	4
Caelo	Lidocaine hydrochloride m...	1808031-03	1
Caelo	Lidocaine hydrochloride m...	1814U-01775	1
Caelo	Lidocaine hydrochloride m...	18179904	19
Caelo	Lidocaine hydrochloride m...	18179905	4
Caelo	Lidocaine hydrochloride m...	18179906	11
Caelo	Lidocaine hydrochloride m...	18179910	8
Caelo	Lidocaine hydrochloride m...	18179911	11
Caelo	Lidocaine hydrochloride m...	18179912	1
Caelo	Lidocaine hydrochloride m...	18179913	1
Caelo	Lidocaine hydrochloride m...	18179914	5
Caelo	Lidocaine hydrochloride m...	18179915	12
Caelo	Lidocaine hydrochloride m...	18179917	1
Caelo	Lidocaine hydrochloride m...	18179922	2
Caelo	Lidocaine hydrochloride m...	18179922/P-06091922	1
Caelo	Lidocaine hydrochloride m...	18179923	4
Caelo	Lidocaine hydrochloride m...	18179924	10
Caelo	Lidocaine hydrochloride m...	18179924P-200319-12	1
Caelo	Lidocaine hydrochloride m...	1819914	1
Caelo	Lidocaine hydrochloride m...	1879904	1
Caelo	Lidocaine hydrochloride m...	18B23-B03	1
Caelo	Lidocaine hydrochloride m...	18B23-B03-347316	1
Caelo	Lidocaine hydrochloride m...	18B23-B03-355046	1
Caelo	Lidocaine hydrochloride m...	18B23-B03-352117	1
Caelo	Lidocaine hydrochloride m...	1907012-01	4
Caelo	Lidocaine hydrochloride m...	1907012-02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lidocaine hydrochloride m…	1907012-03	1
Caelo	Lidocaine hydrochloride m…	1907012-04	1
Caelo	Lidocaine hydrochloride m…	1912M-01775	1
Caelo	Lidocaine hydrochloride m…	1913103	1
Caelo	Lidocaine hydrochloride m…	191350002	14
Caelo	Lidocaine hydrochloride m…	191350004	2
Caelo	Lidocaine hydrochloride m…	191350005	13
Caelo	Lidocaine hydrochloride m…	191350007	3
Caelo	Lidocaine hydrochloride m…	191350008	2
Caelo	Lidocaine hydrochloride m…	191350010	26
Caelo	Lidocaine hydrochloride m…	19135102	1
Caelo	Lidocaine hydrochloride m…	19135103	38
Caelo	Lidocaine hydrochloride m…	19135104	17
Caelo	Lidocaine hydrochloride m…	20004307001	3
Caelo	Lidocaine hydrochloride m…	20004451001	4
Caelo	Lidocaine hydrochloride m…	20004451002	22
Caelo	Lidocaine hydrochloride m…	20004451004	9
Caelo	Lidocaine hydrochloride m…	20004451008	22
Caelo	Lidocaine hydrochloride m…	2004451002	1
Caelo	Lidocaine hydrochloride m…	2021903	1
Caelo	Lidocaine hydrochloride m…	2051301	1
Caelo	Lidocaine hydrochloride m…	20C18-B02-196984	2
Caelo	Lidocaine hydrochloride m…	210025003	1
Caelo	Lidocaine hydrochloride m…	21002505003	7
Caelo	Lidocaine hydrochloride m…	21002505006	6
Caelo	Lidocaine hydrochloride m…	21002505007	8
Caelo	Lidocaine hydrochloride m…	21002505011	2
Caelo	Lidocaine hydrochloride m…	210025505007	1
Caelo	Lidocaine hydrochloride m…	2101034/03	1
Caelo	Lidocaine hydrochloride m…	2101034-01	1
Caelo	Lidocaine hydrochloride m…	2101034-02	1
Caelo	Lidocaine hydrochloride m…	2101034-03	2
Caelo	Lidocaine hydrochloride m…	21101034-03	1
Caelo	Lidocaine hydrochloride m…	21C05-B05-210126	1
Caelo	Lidocaine hydrochloride m…	22003202002	6
Caelo	Lidocaine hydrochloride m…	22003202003	2
Caelo	Lidocaine hydrochloride m…	2201026-01	1
Caelo	Lidocaine hydrochloride m…	2201026-02	2
Caelo	Lidocaine hydrochloride m…	22042003	1
Caelo	Lidocaine hydrochloride m…	2211019-01	1
Caelo	Lidocaine hydrochloride m…	2211o19-01	1
Caelo	Lidocaine hydrochloride m…	23011403	1
Caelo	Lidocaine hydrochloride m…	24071401	1
Caelo	Lidocaine hydrochloride m…	25091202	1
Caelo	Lidocaine hydrochloride m…	26041401	1
Caelo	Lidocaine hydrochloride m…	26051802	1
Caelo	Lidocaine hydrochloride m…	26071303	1
Caelo	Lidocaine hydrochloride m…	280501	1
Caelo	Lidocaine hydrochloride m…	28111812	1
Caelo	Lidocaine hydrochloride m…	29081503	1
Caelo	Lidocaine hydrochloride m…	3071711	1
Caelo	Lidocaine hydrochloride m…	4051703	1
Caelo	Lidocaine hydrochloride m…	4111302	1
Caelo	Lidocaine hydrochloride m…	4111703	1
Caelo	Lidocaine hydrochloride m…	415299506	1
Caelo	Lidocaine hydrochloride m…	5113E-01775	1
Caelo	Lidocaine hydrochloride m…	5211E-01775	1
Caelo	Lidocaine hydrochloride m…	6121706	1
Caelo	Lidocaine hydrochloride m…	812-16001	1
Caelo	Lidocaine hydrochloride m…	AKD14	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Lidocaine hydrochloride m...	LDH/118024	1
Caerlo	Lidocaine hydrochloride m...	13118807	1
Caesar & Lorenz GmbH	Lidocaine hydrochloride m...	16222208	1
Caesar & Lorenz GmbH	Lidocaine hydrochloride m...	18179923	2
Caesar & Lorenz GmbH	Lidocaine hydrochloride m...	19135104	1
Caesar & Lorenz GmbH	Lidocaine hydrochloride m...	2273185	1
Caesar & Loretz GmbH...	Lidocaine hydrochloride m...	18179915	1
Caesar & Loretz GmbH...	Lidocaine hydrochloride m...	19135103	1
Caesar & Loretz GmbH/ AEP	Lidocaine hydrochloride m...	191350002	1
Caesar & Loretz GmbH...	Lidocaine hydrochloride m...	21002505011	2
Caesar & Loretz GmbH...	Lidocaine hydrochloride m...	191350002	1
Caesar & Loretz GmbH/AHD	Lidocaine hydrochloride m...	19135103	2
Caesar & Loretz GmbH/AHD	Lidocaine hydrochloride m...	21002505003	1
Caesar & Loretz GmbH...	Lidocaine hydrochloride m...	21002505006	2
Caesar & Loretz GmbH/Gehe	Lidocaine hydrochloride m...	20004451002	3
Caesar & Loretz GmbH...	Lidocaine hydrochloride m...	18179914	1
Caesar & Loretz GmbH...	Lidocaine hydrochloride m...	191350002	2
Caesar & Loretz GmbH...	Lidocaine hydrochloride m...	191350010	1
Caesar & Loretz GmbH...	Lidocaine hydrochloride m...	20004451002	2
Caesar & Loretz GmbH/Gö	Lidocaine hydrochloride m...	191350010	1
Caesar & Loretz GmbH...	Lidocaine hydrochloride m...	19135103	1
Caesar & Loretz GmbH...	Lidocaine hydrochloride m...	19135103	2
Caesar & Loretz GmbH...	Lidocaine hydrochloride m...	18179914	1
Caesar & Loretz GmbH...	Lidocaine hydrochloride m...	18179917	1
Caesar & Loretz GmbH...	Lidocaine hydrochloride m...	191350010	1
Caesar & Loretz GmbH...	Lidocaine hydrochloride m...	20004451002	2
Caesar & Loretz GmbH...	Lidocaine hydrochloride m...	20004451002	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	13343002	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	15215201	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	1612015-03	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	16222203	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	17292311	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	18179903	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	18179904	4
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	18179905	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	18179906	2
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	18179911	4
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	18179912	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	18179914	4
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	18179916	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	18179922	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	18179923	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	1907012-02	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	191350002	7
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	191350004	3
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	191350005	2
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	191350007	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	191350010	10
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	19135103	6
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	19135104	4
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	20004451002	15
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	20004451004	6
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	20004451008	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	210025050004	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	21002505006	2
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	21002505007	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	21002505008	1
Caesar & Loretz GmbH	Lidocaine hydrochloride m...	22003202003	3
Caesar & Loretz/Anza...	Lidocaine hydrochloride m...	18179906	1
Caesar & Loretz	Lidocaine hydrochloride m...	1612015-01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar u Loretz	Lidocaine hydrochloride m…	13343017	1
Caesar&Loretz GmbH /Anzag	Lidocaine hydrochloride m…	15215303	1
Caesar&Loretz GmbH/ …	Lidocaine hydrochloride m…	17204803	1
Caesar&Loretz GmbH/Anzag	Lidocaine hydrochloride m…	13118803	2
Caeser und Loretz GmbH	Lidocaine hydrochloride m…	181799023	1
Caleo/ Noweda	Lidocaine hydrochloride m…	17204804	1
Caolo	Lidocaine hydrochloride m…	13343008	1
Cealo	Lidocaine hydrochloride m…	20004451008	1
Ensbona/ Sanacorp	Lidocaine hydrochloride m…	1606024-01	1
EuRho / Alliance	Lidocaine hydrochloride m…	1907012-03	1
EuRho / Alliance	Lidocaine hydrochloride m…	2101034-01	1
EuRho / Phönix	Lidocaine hydrochloride m…	2201026-01	1
EuRho / Sanacorp	Lidocaine hydrochloride m…	1907012-04	1
EuRho/ Anzag	Lidocaine hydrochloride m…	2201026-01	3
EuRho/ Jenne	Lidocaine hydrochloride m…	2101034-02	1
Eurho/ Noweda	Lidocaine hydrochloride m…	1808031-01	1
Eurho/ Noweda	Lidocaine hydrochloride m…	1808031-03	2
EuRho/ Phönix	Lidocaine hydrochloride m…	1612015-04	1
EuRho/ Sana	Lidocaine hydrochloride m…	1808031-02	1
EuRho/ VDL	Lidocaine hydrochloride m…	1612015-04	1
EuRho/AHD	Lidocaine hydrochloride m…	1907012-01	1
EuRho/AHD	Lidocaine hydrochloride m…	LDH/720023	2
EuRho/Gehe	Lidocaine hydrochloride m…	2101034-01	3
EuRho/Jenne	Lidocaine hydrochloride m…	1907012-02	1
Eurho/Jenne	Lidocaine hydrochloride m…	1907012-04	1
EuRho/Jenne	Lidocaine hydrochloride m…	2101034-03	1
EuRho/Noweda	Lidocaine hydrochloride m…	1612015-02	2
EuRho/Noweda	Lidocaine hydrochloride m…	2101034-01	1
EuRho/Phoenix	Lidocaine hydrochloride m…	1612015-01	1
EuRho/Phoenix	Lidocaine hydrochloride m…	2201026-02	1
EuRho/Phönix	Lidocaine hydrochloride m…	1808031-01	2
EuRho/Phönix	Lidocaine hydrochloride m…	2101034-01	1
EuRho/Sanacorp	Lidocaine hydrochloride m…	1612015-04	1
EuRho/Sanacorp	Lidocaine hydrochloride m…	1808031-01	3
EuRho/VDL	Lidocaine hydrochloride m…	1612015-03	2
EuRho	Lidocaine hydrochloride m…	1108017-01	3
EuRho	Lidocaine hydrochloride m…	140302501	1
EuRho	Lidocaine hydrochloride m…	1403025-02	1
EuRho	Lidocaine hydrochloride m…	1505023-01	4
EuRho	Lidocaine hydrochloride m…	1505023-02	1
EuRho	Lidocaine hydrochloride m…	1612015-01	2
EuRho	Lidocaine hydrochloride m…	161201502	1
EuRho	Lidocaine hydrochloride m…	1612015-02	1
EuRho	Lidocaine hydrochloride m…	1612015-04	1
EuRho	Lidocaine hydrochloride m…	18008031	1
EuRho	Lidocaine hydrochloride m…	1808031-02	2
EuRho	Lidocaine hydrochloride m…	1808031-03	1
Eurho	Lidocaine hydrochloride m…	1907012-02	1
EuRho	Lidocaine hydrochloride m…	2101034	1
Eurho	Lidocaine hydrochloride m…	2101034-01	1
EuRho	Lidocaine hydrochloride m…	2101034-03	1
Eurho	Lidocaine hydrochloride m…	2101034-04	1
EuRho	Lidocaine hydrochloride m…	2201026-01	1
EuRho	Lidocaine hydrochloride m…	2201026-02	2
EuRho	Lidocaine hydrochloride m…	2211019-01	1
EuRho	Lidocaine hydrochloride m…	EuRho	1
EuRho	Lidocaine hydrochloride m…	LDH720023	1
Euro OTC	Lidocaine hydrochloride m…		4
Euro OTC	Lidocaine hydrochloride m…	1004040-01	1
Euro OTC	Lidocaine hydrochloride m…	1010024-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Lidocaine hydrochloride m...	1066024-01	1
Euro OTC	Lidocaine hydrochloride m...	1103034-01	2
Euro OTC	Lidocaine hydrochloride m...	1108017-01	5
Euro OTC	Lidocaine hydrochloride m...	1108017-02	7
Euro OTC	Lidocaine hydrochloride m...	1140917/160602403	1
Euro OTC	Lidocaine hydrochloride m...	1202034-01	2
Euro OTC	Lidocaine hydrochloride m...	1202035	1
Euro OTC	Lidocaine hydrochloride m...	1202035/02	1
Euro OTC	Lidocaine hydrochloride m...	1202035-01	24
Euro OTC	Lidocaine hydrochloride m...	120203502	3
Euro OTC	Lidocaine hydrochloride m...	1202035-02	35
Euro OTC	Lidocaine hydrochloride m...	1202035-03	11
Euro OTC	Lidocaine hydrochloride m...	1202035-1	1
Euro OTC	Lidocaine hydrochloride m...	12020351612015-01	1
Euro OTC	Lidocaine hydrochloride m...	1401010-01	1
Euro OTC	Lidocaine hydrochloride m...	1403025	1
Euro OTC	Lidocaine hydrochloride m...	140302501	2
Euro OTC	Lidocaine hydrochloride m...	1403025-01	22
Euro OTC	Lidocaine hydrochloride m...	140302502	2
Euro OTC	Lidocaine hydrochloride m...	1403025-02	15
Euro OTC	Lidocaine hydrochloride m...	1403025-03	1
Euro OTC	Lidocaine hydrochloride m...	140415A	1
Euro OTC	Lidocaine hydrochloride m...	141101	1
Euro OTC	Lidocaine hydrochloride m...	141101001	4
Euro OTC	Lidocaine hydrochloride m...	1411010-01	39
Euro OTC	Lidocaine hydrochloride m...	1411010-01Mg25g	1
Euro OTC	Lidocaine hydrochloride m...	141101002	3
Euro OTC	Lidocaine hydrochloride m...	1411010-02	26
Euro OTC	Lidocaine hydrochloride m...	1411010-02Mg50g	1
Euro OTC	Lidocaine hydrochloride m...	141101-01	1
Euro OTC	Lidocaine hydrochloride m...	14110101-01	1
Euro OTC	Lidocaine hydrochloride m...	1411010-2	1
Euro OTC	Lidocaine hydrochloride m...	150502301	3
Euro OTC	Lidocaine hydrochloride m...	1505023-01	71
Euro OTC	Lidocaine hydrochloride m...	1505023-02	21
Euro OTC	Lidocaine hydrochloride m...	1505023-03	16
Euro OTC	Lidocaine hydrochloride m...	150523-02	1
Euro OTC	Lidocaine hydrochloride m...	1512015-04	1
Euro OTC	Lidocaine hydrochloride m...	1600024-02	1
Euro OTC	Lidocaine hydrochloride m...	16006024-02	1
Euro OTC	Lidocaine hydrochloride m...	1606021-01	1
Euro OTC	Lidocaine hydrochloride m...	1606024_02	3
Euro OTC	Lidocaine hydrochloride m...	160602401	3
Euro OTC	Lidocaine hydrochloride m...	1606024-01	67
Euro OTC	Lidocaine hydrochloride m...	160602402	2
Euro OTC	Lidocaine hydrochloride m...	1606024-02	76
Euro OTC	Lidocaine hydrochloride m...	1606024-03	24
Euro OTC	Lidocaine hydrochloride m...	1606024-1	1
Euro OTC	Lidocaine hydrochloride m...	160624-01	1
Euro OTC	Lidocaine hydrochloride m...	16112015-01	2
Euro OTC	Lidocaine hydrochloride m...	16112015-04	1
Euro OTC	Lidocaine hydrochloride m...	1612012015-04	1
Euro OTC	Lidocaine hydrochloride m...	1612015	6
Euro OTC	Lidocaine hydrochloride m...	1612015_01	1
Euro OTC	Lidocaine hydrochloride m...	161201501	1
Euro OTC	Lidocaine hydrochloride m...	1612015-01	51
Euro OTC	Lidocaine hydrochloride m...	161201502	3
Euro OTC	Lidocaine hydrochloride m...	1612015-02	74
Euro OTC	Lidocaine hydrochloride m...	1612015-03	24
Euro OTC	Lidocaine hydrochloride m...	161201504	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Lidocaine hydrochloride m…	1612015-04	36
Euro OTC	Lidocaine hydrochloride m…	1612015-05	3
Euro OTC	Lidocaine hydrochloride m…	1612015-14	1
Euro OTC	Lidocaine hydrochloride m…	16122016-01	1
Euro OTC	Lidocaine hydrochloride m…	1618015-02	1
Euro OTC	Lidocaine hydrochloride m…	168020	2
Euro OTC	Lidocaine hydrochloride m…	170612182	1
Euro OTC	Lidocaine hydrochloride m…	171106LHC/1606024-03	1
Euro OTC	Lidocaine hydrochloride m…	17204803	2
Euro OTC	Lidocaine hydrochloride m…	17204810	1
Euro OTC	Lidocaine hydrochloride m…	180220L/1612015-01	1
Euro OTC	Lidocaine hydrochloride m…	18080031	1
Euro OTC	Lidocaine hydrochloride m…	180803-01	1
Euro OTC	Lidocaine hydrochloride m…	1808031	5
Euro OTC	Lidocaine hydrochloride m…	180803101	4
Euro OTC	Lidocaine hydrochloride m…	1808031-01	119
Euro OTC	Lidocaine hydrochloride m…	1808031-01Retest	1
Euro OTC	Lidocaine hydrochloride m…	180803102	2
Euro OTC	Lidocaine hydrochloride m…	1808031-02	88
Euro OTC	Lidocaine hydrochloride m…	180803103	1
Euro OTC	Lidocaine hydrochloride m…	1808031-03	40
Euro OTC	Lidocaine hydrochloride m…	1808031-04	1
Euro OTC	Lidocaine hydrochloride m…	18908031-01	1
Euro OTC	Lidocaine hydrochloride m…	1907012	2
Euro OTC	Lidocaine hydrochloride m…	1907012_01	1
Euro OTC	Lidocaine hydrochloride m…	190701201	4
Euro OTC	Lidocaine hydrochloride m…	1907012-01	151
Euro OTC	Lidocaine hydrochloride m…	190701202	1
Euro OTC	Lidocaine hydrochloride m…	1907012-02	110
Euro OTC	Lidocaine hydrochloride m…	1907012-03	91
Euro OTC	Lidocaine hydrochloride m…	190701204	1
Euro OTC	Lidocaine hydrochloride m…	1907012-04	62
Euro OTC	Lidocaine hydrochloride m…	1907012-1	3
Euro OTC	Lidocaine hydrochloride m…	1907012-12	1
Euro OTC	Lidocaine hydrochloride m…	1907012-42	1
Euro OTC	Lidocaine hydrochloride m…	1907012-62	1
Euro OTC	Lidocaine hydrochloride m…	1907013-03	1
Euro OTC	Lidocaine hydrochloride m…	190720107	1
Euro OTC	Lidocaine hydrochloride m…	19097012-01	1
Euro OTC	Lidocaine hydrochloride m…	197012-09	1
Euro OTC	Lidocaine hydrochloride m…	20131010-4	1
Euro OTC	Lidocaine hydrochloride m…	20C18-B02-196984	1
Euro OTC	Lidocaine hydrochloride m…	210034-02	1
Euro OTC	Lidocaine hydrochloride m…	2101031-01	1
Euro OTC	Lidocaine hydrochloride m…	2101034	1
Euro OTC	Lidocaine hydrochloride m…	210103401	1
Euro OTC	Lidocaine hydrochloride m…	2101034-01	57
Euro OTC	Lidocaine hydrochloride m…	2101034-02	46
Euro OTC	Lidocaine hydrochloride m…	210103403	1
Euro OTC	Lidocaine hydrochloride m…	2101034-03	38
Euro OTC	Lidocaine hydrochloride m…	2101034-04	7
Euro OTC	Lidocaine hydrochloride m…	2101034-3	1
Euro OTC	Lidocaine hydrochloride m…	2201026	2
Euro OTC	Lidocaine hydrochloride m…	2201026_01	1
Euro OTC	Lidocaine hydrochloride m…	220102601	4
Euro OTC	Lidocaine hydrochloride m…	2201026-01	102
Euro OTC	Lidocaine hydrochloride m…	2201026-02	44
Euro OTC	Lidocaine hydrochloride m…	2201026-1	1
Euro OTC	Lidocaine hydrochloride m…	2201062-01	1
Euro OTC	Lidocaine hydrochloride m…	220126-02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Lidocaine hydrochloride m...	22101901	1
Euro OTC	Lidocaine hydrochloride m...	221019-01	2
Euro OTC	Lidocaine hydrochloride m...	221026-02	1
Euro OTC	Lidocaine hydrochloride m...	221101901	2
Euro OTC	Lidocaine hydrochloride m...	2211019-01	13
Euro OTC	Lidocaine hydrochloride m...	2213U01775	1
Euro OTC	Lidocaine hydrochloride m...	23081601	1
Euro OTC	Lidocaine hydrochloride m...	2805016-01	1
Euro OTC	Lidocaine hydrochloride m...	2810029-01	1
Euro OTC	Lidocaine hydrochloride m...	2886	1
Euro OTC	Lidocaine hydrochloride m...	991011	1
Euro OTC	Lidocaine hydrochloride m...	AP220802-02	1
Euro OTC	Lidocaine hydrochloride m...	ldh/116023	1
Euro OTC	Lidocaine hydrochloride m...	LDH/116023	3
Euro OTC	Lidocaine hydrochloride m...	LDH/118024	4
Euro OTC	Lidocaine hydrochloride m...	LDH/121043	4
Euro OTC	Lidocaine hydrochloride m...	LDH/719007	5
Euro OTC	Lidocaine hydrochloride m...	LDH/720023	2
Euro OTC	Lidocaine hydrochloride m...	LDH/722031	1
Euro OTC	Lidocaine hydrochloride m...	LDHI719007	1
Euro OTC	Lidocaine hydrochloride m...	LDHV121043	1
Euro OTC	Lidocaine hydrochloride m...	lhd719007	1
Euro OTC	Lidocaine hydrochloride m...	LID-20-11-001	2
Euro/ Anzag	Lidocaine hydrochloride m...	1606024-03	1
Euro/ Gehe	Lidocaine hydrochloride m...	1808031-03	1
Euro/ Gehe	Lidocaine hydrochloride m...	1907012-01	2
Euro/ Gehe	Lidocaine hydrochloride m...	1907012-02	1
Euro/ Jenne	Lidocaine hydrochloride m...	1907012-02	1
Euro/Alliance Healthcare	Lidocaine hydrochloride m...	150523-01	1
euro/Gehe	Lidocaine hydrochloride m...	1907012-04	1
Euro/Gehe	Lidocaine hydrochloride m...	2201026-02	1
Euro/Phoenix	Lidocaine hydrochloride m...	1907012-01	3
Euro/Phönix	Lidocaine hydrochloride m...	141101010-01	1
Euro/Phönix	Lidocaine hydrochloride m...	1612015-01	1
Euro/Phönix	Lidocaine hydrochloride m...	1808031-02	1
Euro/Phönix	Lidocaine hydrochloride m...	1808031-03	1
Euro/Phönix	Lidocaine hydrochloride m...	210103401	1
Euro/Phönix	Lidocaine hydrochloride m...	2101034-03	1
Euro/Sanacorp	Lidocaine hydrochloride m...	1808031-03	1
Euro/Sanacorp	Lidocaine hydrochloride m...	2101034-01	1
Euro	Lidocaine hydrochloride m...	1505023-01	2
Europ Ots Pharma	Lidocaine hydrochloride m...	1403025-01	1
EuroPharm	Lidocaine hydrochloride m...	1907012-02	1
Europharm	Lidocaine hydrochloride m...	2101034-02	4
EuroPharm	Lidocaine hydrochloride m...	2101034-02	1
Fagon	Lidocaine hydrochloride m...	15/17-B01-316805	1
Fagron	Lidocaine hydrochloride m...	11H18-N01	1
Fagron	Lidocaine hydrochloride m...	11L09-N09	2
Fagron	Lidocaine hydrochloride m...	1202035-02	1
Fagron	Lidocaine hydrochloride m...	12c05-N02	1
Fagron	Lidocaine hydrochloride m...	12C05-N02	1
Fagron	Lidocaine hydrochloride m...	12E14-N04	2
Fagron	Lidocaine hydrochloride m...	12H09-N08	2
Fagron	Lidocaine hydrochloride m...	13218-B11	1
Fagron	Lidocaine hydrochloride m...	13F07N06	1
Fagron	Lidocaine hydrochloride m...	13F07-N06	7
Fagron	Lidocaine hydrochloride m...	13L18-B11-286901	1
Fagron	Lidocaine hydrochloride m...	14/20-B05	1
Fagron	Lidocaine hydrochloride m...	1420-b05-303	1
Fagron	Lidocaine hydrochloride m...	14B12-B03-292214	9

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Lidocaine hydrochloride m…	14e13-b06-294973	1
Fagron	Lidocaine hydrochloride m…	14e13-b06-294975	2
Fagron	Lidocaine hydrochloride m…	14E13-B06-294975	5
Fagron	Lidocaine hydrochloride m…	14J07-B04-299433	4
Fagron	Lidocaine hydrochloride m…	14J07-B04-299434	2
Fagron	Lidocaine hydrochloride m…	14J20-b05	1
Fagron	Lidocaine hydrochloride m…	14J20-B05-303131	2
Fagron	Lidocaine hydrochloride m…	14j20-b05-303133	1
Fagron	Lidocaine hydrochloride m…	14J20-B05-303133	2
Fagron	Lidocaine hydrochloride m…	15/17-b01-315828	1
Fagron	Lidocaine hydrochloride m…	15/17-B01316805	1
Fagron	Lidocaine hydrochloride m…	15/17-B01-316805	8
Fagron	Lidocaine hydrochloride m…	1505023-01	2
Fagron	Lidocaine hydrochloride m…	1517-801	1
Fagron	Lidocaine hydrochloride m…	1517-B01	1
Fagron	Lidocaine hydrochloride m…	15215311	2
Fagron	Lidocaine hydrochloride m…	15299513	1
Fagron	Lidocaine hydrochloride m…	15299516	1
Fagron	Lidocaine hydrochloride m…	15I17-B01-315828	2
Fagron	Lidocaine hydrochloride m…	15I17-b01-316805	1
Fagron	Lidocaine hydrochloride m…	15I17-B01-316805	2
Fagron	Lidocaine hydrochloride m…	161201501	1
Fagron	Lidocaine hydrochloride m…	1612015-01	1
Fagron	Lidocaine hydrochloride m…	1612015-02	3
Fagron	Lidocaine hydrochloride m…	1612015-03	1
Fagron	Lidocaine hydrochloride m…	168020-0001	1
Fagron	Lidocaine hydrochloride m…	16C09-B03	1
Fagron	Lidocaine hydrochloride m…	16C09-B03-319230	1
Fagron	Lidocaine hydrochloride m…	16c09b03322144	1
Fagron	Lidocaine hydrochloride m…	16C09-B03-322144	4
Fagron	Lidocaine hydrochloride m…	16c09-b03-322145	2
Fagron	Lidocaine hydrochloride m…	16C09-B03-322145	1
Fagron	Lidocaine hydrochloride m…	16J24-B15-329421	1
Fagron	Lidocaine hydrochloride m…	17A16-B07	2
Fagron	Lidocaine hydrochloride m…	17A16-B07-331959	4
Fagron	Lidocaine hydrochloride m…	17A16B07333010	1
Fagron	Lidocaine hydrochloride m…	17A16-B07-333010	4
Fagron	Lidocaine hydrochloride m…	17G10-B08-342287	1
Fagron	Lidocaine hydrochloride m…	17G10-B08-346659	3
Fagron	Lidocaine hydrochloride m…	17G10-B08-346659	1
Fagron	Lidocaine hydrochloride m…	1808031-01	1
Fagron	Lidocaine hydrochloride m…	1808031-02	2
Fagron	Lidocaine hydrochloride m…	1808031-03	1
Fagron	Lidocaine hydrochloride m…	18B23-B03	5
Fagron	Lidocaine hydrochloride m…	18B23-B03_355046	1
Fagron	Lidocaine hydrochloride m…	18B23-B03-347316	5
Fagron	Lidocaine hydrochloride m…	18B23-B03-348590	3
Fagron	Lidocaine hydrochloride m…	18B23-B03-348748	1
Fagron	Lidocaine hydrochloride m…	18B23-B03-352117	4
Fagron	Lidocaine hydrochloride m…	18B23-B03-353035	1
Fagron	Lidocaine hydrochloride m…	18B23-B03-354288	5
Fagron	Lidocaine hydrochloride m…	18B23-B03-355046	1
Fagron	Lidocaine hydrochloride m…	18B23-B03-355381	1
Fagron	Lidocaine hydrochloride m…	18B23-B04-348590	1
Fagron	Lidocaine hydrochloride m…	1907012-02	1
Fagron	Lidocaine hydrochloride m…	19E22-B01-1914608	1
Fagron	Lidocaine hydrochloride m…	19E22-B01-191467	5
Fagron	Lidocaine hydrochloride m…	19E22-B01-191468	9
Fagron	Lidocaine hydrochloride m…	19J16-B02	1
Fagron	Lidocaine hydrochloride m…	19J16-B02-196983	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Lidocaine hydrochloride m...	19j16-b02-196985	1
Fagron	Lidocaine hydrochloride m...	19J16-B02-196993	2
Fagron	Lidocaine hydrochloride m...	19J16-BO2-196983	2
Fagron	Lidocaine hydrochloride m...	20A31-B06	2
Fagron	Lidocaine hydrochloride m...	20A31-B06-196986	1
Fagron	Lidocaine hydrochloride m...	20A31-B06-2005105	1
Fagron	Lidocaine hydrochloride m...	20A31-B06-200515	6
Fagron	Lidocaine hydrochloride m...	20C18B02	1
Fagron	Lidocaine hydrochloride m...	20C18-B02	1
Fagron	Lidocaine hydrochloride m...	20c18-b02-196984	1
Fagron	Lidocaine hydrochloride m...	20C18-B02-196984	9
Fagron	Lidocaine hydrochloride m...	20E28-B04-201210	1
Fagron	Lidocaine hydrochloride m...	20e28-b04-201268	1
Fagron	Lidocaine hydrochloride m...	20E28-B04-201302	1
Fagron	Lidocaine hydrochloride m...	20E28-B04-201702	3
Fagron	Lidocaine hydrochloride m...	20E28-B04-2017021	1
Fagron	Lidocaine hydrochloride m...	21/17-803-216827	1
Fagron	Lidocaine hydrochloride m...	21/17-B03-216798	2
Fagron	Lidocaine hydrochloride m...	21/17-B03-216827	1
Fagron	Lidocaine hydrochloride m...	218I-01775	1
Fagron	Lidocaine hydrochloride m...	21A12B04203052	1
Fagron	Lidocaine hydrochloride m...	21A12-B04-203052	2
Fagron	Lidocaine hydrochloride m...	21C05-B05-210126	1
Fagron	Lidocaine hydrochloride m...	21I17-B03	1
Fagron	Lidocaine hydrochloride m...	21I17-B03-213766	2
Fagron	Lidocaine hydrochloride m...	21I17-B03-213769	4
Fagron	Lidocaine hydrochloride m...	21I17-B03-216798	1
Fagron	Lidocaine hydrochloride m...	21I17-BO3	1
Fagron	Lidocaine hydrochloride m...	21l17-B03-213769	1
Fagron	Lidocaine hydrochloride m...	2201026-01	1
Fagron	Lidocaine hydrochloride m...	22C15-B16	1
Fagron	Lidocaine hydrochloride m...	22C15-B16-218866	1
Fagron	Lidocaine hydrochloride m...	22C15-B16-220955	2
Fagron	Lidocaine hydrochloride m...	22H22-B03-224257	1
Fagron	Lidocaine hydrochloride m...	4612Q-01775	1
Fagron	Lidocaine hydrochloride m...	812-16001	3
Fagron	Lidocaine hydrochloride m...	8F26-N07	1
Fagron	Lidocaine hydrochloride m...	9B3M1L2Fo118	1
Fagron	Lidocaine hydrochloride m...	9E08-N03	1
Fagron	Lidocaine hydrochloride m...	B01-1914608	1
Fagron	Lidocaine hydrochloride m...	B02-1969803	1
Fagron	Lidocaine hydrochloride m...	B02-1969804	3
Fagron	Lidocaine hydrochloride m...	B03-2167908	1
Fagron	Lidocaine hydrochloride m...	B04-2030502	2
Fagron	Lidocaine hydrochloride m...	LDH/116023	1
Fagron	Lidocaine hydrochloride m...	LDH/116037	2
Fagron	Lidocaine hydrochloride m...	LDH/117022	1
Fagron	Lidocaine hydrochloride m...	LDH/117049	1
Fagron	Lidocaine hydrochloride m...	LDH/118024	1
Fagron	Lidocaine hydrochloride m...	LDH/119022	1
Fagron	Lidocaine hydrochloride m...	LDH-721013	1
Fargon GmbH & Co.KG	Lidocaine hydrochloride m...	15/17-B01-316805	1
Fargon GmbH & Co.KG	Lidocaine hydrochloride m...	16C09-B03-322144	2
Fargon	Lidocaine hydrochloride m...	20C18-B02-196948	1
fargon	Lidocaine hydrochloride m...	720005	1
Fiebig 04.7.13 EK 4,54	Lidocaine hydrochloride m...	12135511	1
Fiebig	Lidocaine hydrochloride m...	1808031-01	1
Fiebig	Lidocaine hydrochloride m...	1907012-01	1
Fiebig	Lidocaine hydrochloride m...	20C18-B02-196984	1
Finze	Lidocaine hydrochloride m...	1202035-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Frago/Noweda	Lidocaine hydrochloride m…	6108-05-0	1
Gatt-Koller	Lidocaine hydrochloride m…	1801084	1
Gehe amax	Lidocaine hydrochloride m…	17292308	1
Gehe amax	Lidocaine hydrochloride m…	19135103	1
Gehe Rostock	Lidocaine hydrochloride m…	2201026-01	1
Gehe/EuRho	Lidocaine hydrochloride m…	1907012-02	1
Gehe/Euro	Lidocaine hydrochloride m…	1612015-02	1
Gehe	Lidocaine hydrochloride m…	1190313	1
Gehe	Lidocaine hydrochloride m…	1202035-02	1
Gehe	Lidocaine hydrochloride m…	12C05-N02	2
Gehe	Lidocaine hydrochloride m…	1411010-01	1
Gehe	Lidocaine hydrochloride m…	141101002	1
Gehe	Lidocaine hydrochloride m…	15215304	1
Gehe	Lidocaine hydrochloride m…	15299513	1
Gehe	Lidocaine hydrochloride m…	15299516	1
Gehe	Lidocaine hydrochloride m…	1606024-02	1
GEHE	Lidocaine hydrochloride m…	1606024-02	1
Gehe	Lidocaine hydrochloride m…	1612015-01	1
GEHE	Lidocaine hydrochloride m…	1612015-01	1
Gehe	Lidocaine hydrochloride m…	1612015-02	2
GEHE	Lidocaine hydrochloride m…	1612015-02	1
Gehe	Lidocaine hydrochloride m…	16222207	1
GEHE	Lidocaine hydrochloride m…	16222214	1
GEHE	Lidocaine hydrochloride m…	17292312	1
Gehe	Lidocaine hydrochloride m…	1808031-01	1
Gehe	Lidocaine hydrochloride m…	1808031-02	1
Gehe	Lidocaine hydrochloride m…	18179904	1
Gehe	Lidocaine hydrochloride m…	1907012-01	5
Gehe	Lidocaine hydrochloride m…	1907012-02	2
Gehe	Lidocaine hydrochloride m…	1907012-03	1
Gehe	Lidocaine hydrochloride m…	191350002	2
Gehe	Lidocaine hydrochloride m…	191350007	1
Gehe	Lidocaine hydrochloride m…	2101034-01	1
Gehe	Lidocaine hydrochloride m…	2201026-01	1
Gehe	Lidocaine hydrochloride m…	2201026-02	4
Gehe	Lidocaine hydrochloride m…	221026-01	1
Gehe	Lidocaine hydrochloride m…	2211019-01	4
Gehe	Lidocaine hydrochloride m…	23003452004	1
Gehe	Lidocaine hydrochloride m…	LDH/116023	1
Gehe	Lidocaine hydrochloride m…	LDH/719007	1
Geibo/EuRho	Lidocaine hydrochloride m…	1515023-01	1
Geibo/Euro 29.8.	Lidocaine hydrochloride m…	1808031-02	1
GMP Konform	Lidocaine hydrochloride m…	20A31-B06	1
Hänseler	Lidocaine hydrochloride m…		3
Hedinger/Ebert	Lidocaine hydrochloride m…	13118807	1
INTERN-DROGEN	Lidocaine hydrochloride m…	20004451008	1
INTERN-DROGEN	Lidocaine hydrochloride m…	21002505006	1
Jenne	Lidocaine hydrochloride m…	1808031-02	1
Jenne	Lidocaine hydrochloride m…	1907012-04	1
Jenne	Lidocaine hydrochloride m…	2101034-02	1
Kehr/EuRho	Lidocaine hydrochloride m…	1907012-03	1
Kehr	Lidocaine hydrochloride m…	1606024-02	1
Kehr	Lidocaine hydrochloride m…	1612015-01	1
Kehr	Lidocaine hydrochloride m…	1612015-02	1
Kehr	Lidocaine hydrochloride m…	1612015-03	1
Kehr	Lidocaine hydrochloride m…	21002505007	1
Kehr	Lidocaine hydrochloride m…	22003202003	1
Kehr	Lidocaine hydrochloride m…	22003202007	1
Klenk	Lidocaine hydrochloride m…	1612015-01	2
kögl	Lidocaine hydrochloride m…	1803832	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Konduskar/Phönix	Lidocaine hydrochloride m...	1202035-03	1
Krieger	Lidocaine hydrochloride m...	1612015-04	1
L10	Lidocaine hydrochloride m...	1612015-01	1
L10	Lidocaine hydrochloride m...	1612015-03	1
L12	Lidocaine hydrochloride m...	1505023-02	1
L12	Lidocaine hydrochloride m...	1606024-01	2
Lamotte/Noweda	Lidocaine hydrochloride m...	1622207	1
Mahendra Chem./ Phön...	Lidocaine hydrochloride m...	1411010-01	1
Mahendra Chem./Noweda	Lidocaine hydrochloride m...	1505023	1
Mahendra Chem.	Lidocaine hydrochloride m...	1411010-01	1
Merck	Lidocaine hydrochloride m...	K52817248	1
Moehns BCN, S.L.	Lidocaine hydrochloride m...	191350002	1
Moehs / Ebert	Lidocaine hydrochloride m...	15215201	1
Moehs / Gehe	Lidocaine hydrochloride m...	17292313	1
Moehs Catalana, S.L....	Lidocaine hydrochloride m...		1
Noweda 04.12.2019	Lidocaine hydrochloride m...	907012-01	1
Noweda 23.10.2019	Lidocaine hydrochloride m...	1808031-03	1
Noweda/apotec	Lidocaine hydrochloride m...	2201026-01	1
Noweda/Eurho 18,01,2...	Lidocaine hydrochloride m...	1907012-03	1
Noweda/EuRho	Lidocaine hydrochloride m...	2101034-03	1
Noweda/EuRo	Lidocaine hydrochloride m...	1612015-03	1
Noweda	Lidocaine hydrochloride m...	1108017-02	1
Noweda	Lidocaine hydrochloride m...	1202035-03	1
Noweda	Lidocaine hydrochloride m...	141101002	1
Noweda	Lidocaine hydrochloride m...	1606024-01	1
Noweda	Lidocaine hydrochloride m...	1606024-02	1
Noweda	Lidocaine hydrochloride m...	1612015-02	1
Noweda	Lidocaine hydrochloride m...	1612015-05	1
Noweda	Lidocaine hydrochloride m...	16222207	2
Noweda	Lidocaine hydrochloride m...	16222214	1
Noweda	Lidocaine hydrochloride m...	17204804	1
Noweda	Lidocaine hydrochloride m...	17292304	1
Noweda	Lidocaine hydrochloride m...	1808031-01	1
Noweda	Lidocaine hydrochloride m...	1808031-02	2
Noweda	Lidocaine hydrochloride m...	1808031-03	1
Noweda	Lidocaine hydrochloride m...	1812015-04	1
Noweda	Lidocaine hydrochloride m...	18179904	2
Noweda	Lidocaine hydrochloride m...	1907012_02	1
Noweda	Lidocaine hydrochloride m...	1907012-01	2
Noweda	Lidocaine hydrochloride m...	1907012-02	1
Noweda	Lidocaine hydrochloride m...	1907012-04	1
Noweda	Lidocaine hydrochloride m...	1913500010	1
Noweda	Lidocaine hydrochloride m...	191350007	2
Noweda	Lidocaine hydrochloride m...	20004451004	1
Noweda	Lidocaine hydrochloride m...	20004451008	1
Noweda	Lidocaine hydrochloride m...	2101034-01	2
Noweda	Lidocaine hydrochloride m...	2101034-02	1
Noweda	Lidocaine hydrochloride m...	22003202002	1
Noweda	Lidocaine hydrochloride m...	22003202007	2
Noweda	Lidocaine hydrochloride m...	2201026-01	1
Noweda	Lidocaine hydrochloride m...	2201026-02	1
Noweda	Lidocaine hydrochloride m...	2203202002	1
Noweda	Lidocaine hydrochloride m...	22102601	1
Noweda	Lidocaine hydrochloride m...	2211019-01	2
Noweda	Lidocaine hydrochloride m...	2211019-02	1
Noweda	Lidocaine hydrochloride m...	2273185	1
Noweda	Lidocaine hydrochloride m...	4914889	1
Noweda_31.07.2019	Lidocaine hydrochloride m...	1808031-02	1
Otto G. Apotec	Lidocaine hydrochloride m...	1907012-01	1
Otto Geilenkirchen Aachen	Lidocaine hydrochloride m...	20004307001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Parthe Apotheke	Lidocaine hydrochloride m…	192/20	1
Ph.Eur.10.0/Gehe	Lidocaine hydrochloride m…	1907012-02	1
Phoenix 03.12.2018	Lidocaine hydrochloride m…	1808031-01	1
PHOENIX 17.06.2014	Lidocaine hydrochloride m…	1403025-01	1
Phoenix 26.02.2014	Lidocaine hydrochloride m…	13118814	1
PHOENIX am 12.02.2014	Lidocaine hydrochloride m…	1202035-02	1
Phoenix	Lidocaine hydrochloride m…	1606024-02	1
Phoenix	Lidocaine hydrochloride m…	1612015-02	1
Phoenix	Lidocaine hydrochloride m…	16C09-B03-322144	1
Phoenix	Lidocaine hydrochloride m…	1808031-01	1
Phoenix	Lidocaine hydrochloride m…	1808031-02	3
Phoenix	Lidocaine hydrochloride m…	1808031-03	1
Phoenix	Lidocaine hydrochloride m…	1907012-01	3
Phoenix	Lidocaine hydrochloride m…	1907012-03	1
Phoenix	Lidocaine hydrochloride m…	1907012-04	1
Phoenix	Lidocaine hydrochloride m…	19e22-b01-191467	1
Phoenix	Lidocaine hydrochloride m…	200122101	1
Phoenix	Lidocaine hydrochloride m…	200562306	1
Phoenix	Lidocaine hydrochloride m…	2101034-01	1
Phoenix	Lidocaine hydrochloride m…	2101034-02	1
Phoenix	Lidocaine hydrochloride m…	2101034-03	1
Phoenix	Lidocaine hydrochloride m…	2201026-02	1
Phoenix	Lidocaine hydrochloride m…	2211019-01	2
Phoenix	Lidocaine hydrochloride m…	3238	1
Phönix Gotha	Lidocaine hydrochloride m…	1411010-02	1
Phönix/apo ident	Lidocaine hydrochloride m…	1808031-01	1
Phönix/EuRo	Lidocaine hydrochloride m…	1907012-03	1
Phönix	Lidocaine hydrochloride m…	1202035-03	1
Phönix	Lidocaine hydrochloride m…	12176103	1
phönix	Lidocaine hydrochloride m…	1505023-03	1
Phönix	Lidocaine hydrochloride m…	1606024-01	2
Phönix	Lidocaine hydrochloride m…	1612015-01	2
Phönix	Lidocaine hydrochloride m…	1612015-03	2
phönix	Lidocaine hydrochloride m…	16222207	2
Phönix	Lidocaine hydrochloride m…	1808031-02	1
Phönix	Lidocaine hydrochloride m…	18179904	1
Phönix	Lidocaine hydrochloride m…	1907012-01	3
Phönix	Lidocaine hydrochloride m…	1907012-02	4
PHÖNIX	Lidocaine hydrochloride m…	1907012-02	1
Phönix	Lidocaine hydrochloride m…	190701203	1
Phönix	Lidocaine hydrochloride m…	1907012-03	1
Phönix	Lidocaine hydrochloride m…	20004451002	1
Phönix	Lidocaine hydrochloride m…	21002505007	1
Phönix	Lidocaine hydrochloride m…	2101034-01	1
Phönix	Lidocaine hydrochloride m…	2101034-02	3
Phönix	Lidocaine hydrochloride m…	221019-01	1
Phönix	Lidocaine hydrochloride m…	2211019-02	1
Phönix	Lidocaine hydrochloride m…	B02-1969804	1
Phönix	Lidocaine hydrochloride m…	LDH/722031	1
Rondell Apotheke	Lidocaine hydrochloride m…	15215308	1
sana	Lidocaine hydrochloride m…	1403025-02	1
Sana	Lidocaine hydrochloride m…	2101034-03	1
Sanacorp	Lidocaine hydrochloride m…	1202035-01	3
Sanacorp	Lidocaine hydrochloride m…	13118807	1
Sanacorp	Lidocaine hydrochloride m…	1403025-01	1
Sanacorp	Lidocaine hydrochloride m…	1411010-01	1
Sanacorp	Lidocaine hydrochloride m…	14J07-B04-299434	2
Sanacorp	Lidocaine hydrochloride m…	150502302	1
Sanacorp	Lidocaine hydrochloride m…	15215309	1
Sanacorp	Lidocaine hydrochloride m…	15215312	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Lidocaine hydrochloride m…	15299513	1
Sanacorp	Lidocaine hydrochloride m…	1606024-02	1
Sanacorp	Lidocaine hydrochloride m…	17204804	1
Sanacorp	Lidocaine hydrochloride m…	17292307	1
Sanacorp	Lidocaine hydrochloride m…	17292313	1
Sanacorp	Lidocaine hydrochloride m…	1808031-02	1
Sanacorp	Lidocaine hydrochloride m…	18179911	1
Sanacorp	Lidocaine hydrochloride m…	18179914	1
Sanacorp	Lidocaine hydrochloride m…	19135103	5
Sanacorp	Lidocaine hydrochloride m…	2101034-01	1
Sanacorp	Lidocaine hydrochloride m…	21I17-B03-213766	1
Sanacorp	Lidocaine hydrochloride m…	22003202008	1
Sanacorp	Lidocaine hydrochloride m…	2201023-02	1
Sanacorp	Lidocaine hydrochloride m…	2201026-01	2
Sanacorp	Lidocaine hydrochloride m…	2211019-01	1
Sanacorp	Lidocaine hydrochloride m…	2211019-03	2
Sanacorp	Lidocaine hydrochloride m…	22H22-B03-224257	1
Sanacorp	Lidocaine hydrochloride m…	23003452002	1
Sanacorp	Lidocaine hydrochloride m…	23003452004	1
siehe Protokoll	Lidocaine hydrochloride m…	1606024-01	1
Swati / Noweda	Lidocaine hydrochloride m…	1606024-01	1
Swati /Nowreda	Lidocaine hydrochloride m…	1907012-03	1
Swati Spentose Priva…	Lidocaine hydrochloride m…	1808031-01	1
swati spentose priva…	Lidocaine hydrochloride m…	210103401	1
Swati Spentose Priva…	Lidocaine hydrochloride m…	1907012-04	1
Swati Spentose Private	Lidocaine hydrochloride m…	2101034-01	1
Swati Spentose Private	Lidocaine hydrochloride m…	2101034-02	1
Swati/Noweda	Lidocaine hydrochloride m…	LDH/116007	1
SWATI/Noweda	Lidocaine hydrochloride m…	LDH719007	1
SWATI/Phoenix	Lidocaine hydrochloride m…	LDH/719007	6
SWATI/Phoenix	Lidocaine hydrochloride m…	LDH/720023	3
Swati/Phönix	Lidocaine hydrochloride m…	21A12-B04-203052	1
SWATI/Phönix	Lidocaine hydrochloride m…	LDH/719007	1
Swati/Sanacorp	Lidocaine hydrochloride m…	2201026-01	1
Swati	Lidocaine hydrochloride m…	1606024-01	1
Symbiotica	Lidocaine hydrochloride m…	1606024-02	1

- 232 408 spectra from 1515 *Apo-Ident* customers from a total of 48 770 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Lidocaine hydrochloride monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lidocaine hydrochloride monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	620	0	201 464
Type C	0	3650	9	232 408

The substance/substance group *Lidocaine hydrochloride monohydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0323 %)
Type C	100.0000 % (> 99.9007 %)	99.7540 % (> 99.6720 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20882	20882	0.00	192.57
21613	23807	8.97	188.22
21770	21770	0.00	198.52
23807	23807	0.00	193.87
24776	24776	0.00	202.28
25446	21770	11.40	204.54
26028	26028	0.00	211.62

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Lithium orotate monohydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21055-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lithium orotate monohydrate; Lithii orotas monohydricum

Special notes

When selecting the *Lithium orotate monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Lithium orotate monohydrate	9	9	4

Second-stage model

For differentiation of the substance/substance group *Lithium orotate monohydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Lithium orotate monohydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Oxytetracycline hydrochloride	98.43	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Lithium orotate monohydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Lithium orotate monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Lithium orotate monohydrate	2009002	25404	40	20201020*
Euro OTC	Lithium orotate monohydrate	2102007	25523	40	20210222*
Euro OTC	Lithium orotate monohydrate	2210011	26431	40	20221107*
Euro OTC	Lithium orotate monohydrate	2210011	26431SI	20	20221107*
Euro OTC	Lithium orotate monohydrate	2403013	27207	40	20240508*
Fagron	Lithium orotate monohydrate	13J04-N01	21055	40	1405616
Fagron	Lithium orotate monohydrate	13I09-B04-290311	21688	60	20130927
Fagron	Lithium orotate monohydrate	15F25-B01-315219	22502	40	20150716
Fagron	Lithium orotate monohydrate	18K21-B01-363417	25063	40	20181231
Fagron	Lithium orotate monohydrate	22B26-B12-227899	26541	40	20220608
Fagron	Lithium orotate monohydrate	22B26-B12-227899	26541SI	20	20220608

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 420 spectra of 11 reference samples from the substance/substance group *Lithium orotate monohydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 542 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 380 spectra of 10 reference samples from the substance/substance group *Lithium orotate monohydrate*.

- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Lithium orotate monohydrate	2002030	25146	40
Euro OTC	Lithium orotate monohydrate	2110013	25882	50
Euro OTC	Lithium orotate monohydrate	2311026	26994	40
Euro OTC	Lithium orotate monohydrate	2311003	26995	40
Euro OTC	Lithium orotate monohydrate	2407006	27351	40
Euro OTC	Lithium orotate monohydrate	2408005	27352	40
Euro OTC	Lithium orotate monohydrate	2408006	27353	40
Fagron	Lithium orotate monohydrate	16D15-B08-321402	23269	40
Fagron	Lithium orotate monohydrate	18A19-B12-347442	24111	40
Euro OTC	Lithium orotate monohydrate	2110013	25882SI	10

- 201 704 spectra from a total of 4036 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 7 spectra from 4 *Apo-Ident* customers from 5 batches from the substance/substance group *Lithium orotate monohydrate*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Lithium orotate monohydrate	23K07-B10-232375	1
	Lithium orotate monohydrate	2408005-01	2
AHD	Lithium orotate monohydrate	2407006-01	1
Euro OTC	Lithium orotate monohydrate	2408005-01	1
Fagron	Lithium orotate monohydrate	13J04-N01	1
Pfannenschmidt	Lithium orotate monohydrate	ORL00212	1

- 236 060 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Lithium orotate monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lithium orotate monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	380	0	201 704
Type C	0	7	0	236 060

The substance/substance group *Lithium orotate monohydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.4211 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21055	21055	0.00	193.11
21688	21055	5.84	190.86
22502	21055	8.71	192.10
25063	25523	5.49	191.42
25404	25404	0.00	188.12
25523	25523	0.00	189.03
26431	26431	0.00	193.20
26541	25404	6.43	190.46
27207	27207	0.00	188.65

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**L-Phenylalanine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21661-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

L-Phenylalanine; DL-Phenylalanine; Phenylalanine; Phenylalaninum

Special notes

When selecting the *L-Phenylalanine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
L-Phenylalanine	7	6	4

Second-stage model

For differentiation of the substance/substance group *L-Phenylalanine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *L-Phenylalanine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Amphetamine sulfate	91.46	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *L-Phenylalanine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *L-Phenylalanine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	L-Phenylalanine	14088304	21661	60	1501656
Euro OTC	L-Phenylalanine	1212014-03	21681	60	20130111
Euro OTC	L-Phenylalanine	1704003	23173	40	20170425*
Euro OTC	L-Phenylalanine	2307036	26861	40	20230823*
Euro OTC	L-Phenylalanine	2307036	26861SI	20	20230823*
Fagron	L-Phenylalanine	17B13-B03-343288	23936	40	20170309
Fagron	L-Phenylalanine	19J23-F10-366142	24951	40	20191127
Fagron	L-Phenylalanine	23C07-B05-227911	26671	40	20230327
Fagron	L-Phenylalanine	23C07-B05-227911	26671SI	20	20230327

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *L-Phenylalanine*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 602 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 270 spectra of 7 reference samples from the substance/substance group *L-Phenylalanine*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	L-Phenylalanine	1409013-02	23024	40
Euro OTC	L-Phenylalanine	1808022	24198	40
Euro OTC	L-Phenylalanine	1907032	24846	40
Euro OTC	L-Phenylalanine	2006038	25306	40
Euro OTC	L-Phenylalanine	2105010	25711	50
Euro OTC	L-Phenylalanine	2306009	26871	40
Euro OTC	L-Phenylalanine	2306009	26871SI	20

- 201 814 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 15 spectra from 7 *Apo-Ident* customers from 4 batches from the substance/substance group *L-Phenylalanine*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	L-Phenylalanine	1409013-02	12
Euro OTC	L-Phenylalanine	1704003-02	1
Euro OTC	L-Phenylalanine	200603801	1
Euro OTC	L-Phenylalanine	2006038-01	1

- 236 052 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *L-Phenylalanine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *L-Phenylalanine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	270	0	201 814
Type C	0	15	0	236 052

The substance/substance group *L-Phenylalanine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.7778 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21661	21661	0.00	134.90
21681	21661	25.17	167.33
23173	23173	0.00	199.96

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23936	21661	6.39	135.06
24951	21661	9.09	132.75
26671	21661	7.95	128.95
26861	26861	0.00	152.55

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**L-Threonine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20734-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

L-Threonine; Threonine; Threoninum

Special notes

When selecting the *L-Threonine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
L-Threonine	7	8	4

Second-stage model

For differentiation of the substance/substance group *L-Threonine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *L-Threonine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
5-aminolevulinic acid hydrochloride	78.62	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *L-Threonine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *L-Threonine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	L-Threonine	1210027-01	21033	40	1403152
Euro OTC	L-Threonine	1210027-01	22319	60	20121108
Euro OTC	L-Threonine	1601031	22378	40	20160225*
Euro OTC	L-Threonine	1909003	24850	40	20190913*
Euro OTC	L-Threonine	2004005	25145	40	20200506*
Euro OTC	L-Threonine	2011021	25468	40	20201210*
Euro OTC	L-Threonine	2304006	26643	40	20230510*
Euro OTC	L-Threonine	2304006	26643SI	20	20230510*
Fagron	L-Threonine	12H02-N03	20734	40	1402580

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *L-Threonine*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 602 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 350 spectra of 10 reference samples from the substance/substance group *L-Threonine*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	L-Threonine	1606019	22679	40
Euro OTC	L-Threonine	1609014	22792	40
Euro OTC	L-Threonine	1703035	23158	40
Euro OTC	L-Threonine	1711010	23738	40
Euro OTC	L-Threonine	1811030	24417	40
Euro OTC	L-Threonine	2201020	25946	40
Euro OTC	L-Threonine	2208023	26522	40
Euro OTC	L-Threonine	2404016	27279	40
Euro OTC	L-Threonine	2201020	25946SI	10
Euro OTC	L-Threonine	2208023	26522SI	20

- 201 734 spectra from a total of 4037 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 4 *Apo-Ident* customers from 4 batches from the substance/substance group *L-Threonine*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	L-Threonine	1606019-02	1
Euro OTC	L-Threonine	1811030-01	1
Euro OTC	L-Threonine	2011021-01	1
Fargon	L-Threonine	2114720407	1

- 236 063 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *L-Threonine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *L-Threonine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	350	0	201 734
Type C	0	4	0	236 063

The substance/substance group *L-Threonine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.2857 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20734	20734	0.00	137.08
21033	21033	0.00	135.50
22319	25468	10.68	137.04

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22378	22378	0.00	138.01
24850	24850	0.00	136.10
25145	25145	0.00	141.57
25468	25468	0.00	134.86
26643	26643	0.00	138.08

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Lysine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20385-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Lysine hydrochloride; Lysine HCl; Lysini hydrochloridum

Special notes

When selecting the *Lysine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Lysine hydrochloride	8	11	8

Second-stage model

For differentiation of the substance/substance group *Lysine hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Lysine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Levocarnitine	95.78	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Lysine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Lysine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Lysine hydrochloride	1611021	22865	40	20161202*
Euro OTC	Lysine hydrochloride	1708009	23698	40	20170922*
Euro OTC	Lysine hydrochloride	1805030	24123	40	20180611*
Euro OTC	Lysine hydrochloride	2003009	25128	40	20200403*
Euro OTC	Lysine hydrochloride	2010008	25459	40	20201124*
Euro OTC	Lysine hydrochloride	2105002	25675	40	20210527*
Fagron	Lysine hydrochloride	15B09-B06-304170	21963	60	20150220
Fagron	Lysine hydrochloride	14H20-B03-301894	21983	60	AR-16-FG-005856-01

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 360 spectra of 8 reference samples from the substance/substance group *Lysine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 602 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 500 spectra of 14 reference samples from the substance/substance group *Lysine hydrochloride*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Lysine hydrochloride	1603011	22527	40
Euro OTC	Lysine hydrochloride	1902008	24622	40
Euro OTC	Lysine hydrochloride	1907038	24809	40
Euro OTC	Lysine hydrochloride	2006008	25352	40
Euro OTC	Lysine hydrochloride	2205013	26197	40
Euro OTC	Lysine hydrochloride	2302003	26657	40
Euro OTC	Lysine hydrochloride	2406017	27368	40
Fagron	Lysine hydrochloride	12B14-N08	20735	40
Fagron	Lysine hydrochloride	22J11-B06	26448	40
Fagron	Lysine hydrochloride	23E18-B02-231717	26821	40
Fagron	Lysine hydrochloride	24E06-B24-238724	27413	40
Euro OTC	Lysine hydrochloride	2205013	26197SI	20
Euro OTC	Lysine hydrochloride	2302003	26657SI	20
Fagron	Lysine hydrochloride	23E18-B02-231717	26821SI	20

- 201 584 spectra from a total of 4034 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 22 spectra from 4 *Apo-Ident* customers from 9 batches from the substance/substance group *Lysine hydrochloride*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Lysine hydrochloride	1708009-01	2
Euro OTC	Lysine hydrochloride	1805030-01	1
Euro OTC	Lysine hydrochloride	1907038-01	1
Euro OTC	Lysine hydrochloride	2006008-01	11
Euro OTC	Lysine hydrochloride	2105002-02	2
Euro OTC	Lysine hydrochloride	2205013-01	2
Euro OTC	Lysine hydrochloride	gjjhgjhkj	1
Fagron	Lysine hydrochloride	14H20-B03-301894	1
Fagron	Lysine hydrochloride	21H23-B03-213624	1

- 236 045 spectra from 1515 *Apo-Ident* customers from a total of 49 251 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Lysine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Lysine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	460	40	201 584
Type C	0	22	0	236 045

The substance/substance group *Lysine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	92.0000 % (> 91.4000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 72.7273 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21963	21983	6.75	203.00
21983	21983	0.00	203.13
22865	22865	0.00	198.14
23698	23698	0.00	201.92
24123	24123	0.00	198.55
25128	25128	0.00	203.75
25459	25459	0.00	195.01
25675	25675	0.00	146.61

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Macrogols 1500**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20112-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Macrogols 1500; Macrogolum 1500

Special notes

When selecting the *Macrogols 1500* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Macrogols 1500	9	6	45

Second-stage model

For differentiation of the substance/substance group *Macrogols 1500* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Macrogols 1500* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Macrogols 4000	36.90	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Macrogols 1500* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Macrogols 1500*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Macrogols 1500	12324607	20977	40	1403323
Caelo	Macrogols 1500	17120001	23241	40	20170519
Caelo	Macrogols 1500	171200	23291	40	20170519*
Caelo	Macrogols 1500	21003420001	25988	40	20220103
Caelo	Macrogols 1500	21003420001	25988SI	30	20220103
Caelo	Macrogols 1500	24001044	27236	40	20240618*
Caelo	Macrogols 1500	24001044	27236SI	20	20240618*
Caelo	Macrogols 1500	24001643	27323	40	20240808*
Caelo	Macrogols 1500	24001643	27323SI	20	20240808*
Euro OTC	Macrogols 1500	1508002	21948	60	20150810*
Euro OTC	Macrogols 1500	1604005	22544	40	20160512*
Euro OTC	Macrogols 1500	2009003	25302	40	20200916*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 450 spectra of 12 reference samples from the substance/substance group *Macrogols 1500*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 512 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 6 reference samples from the substance/substance group *Macrogols 1500*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Macrogols 1500	172221	23625	40
Caelo	Macrogols 1500	182290	24350	40
Euro OTC	Macrogols 1500	1705004	23423	40
Euro OTC	Macrogols 1500	1705036	23440	40
Euro OTC	Macrogols 1500	1711032	23898	40
Euro OTC	Macrogols 1500	1806015	24147	40

- 201 844 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 85 spectra from 36 *Apo-Ident* customers from 47 batches from the substance/substance group *Macrogols 1500*.

- Among them are spectra of independent samples from 45 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
ACM / Herba	Macrogols 1500	KN-0826/10	1
Caelo	Macrogols 1500	10105901	1
Caelo	Macrogols 1500	11071309	1
Caelo	Macrogols 1500	12109409	1
Caelo	Macrogols 1500	13140901	1
Caelo	Macrogols 1500	13140902	2
Caelo	Macrogols 1500	13140906	1
Caelo	Macrogols 1500	14072409	1
Caelo	Macrogols 1500	14072412	1
Caelo	Macrogols 1500	15120007	1
Caelo	Macrogols 1500	1513101	1
Caelo	Macrogols 1500	15413101	2
Caelo	Macrogols 1500	15413104	1
Caelo	Macrogols 1500	15413105	5
Caelo	Macrogols 1500	15413111	2
Caelo	Macrogols 1500	16138407	1
Caelo	Macrogols 1500	17120001	3
Caelo	Macrogols 1500	17120002	2
Caelo	Macrogols 1500	17120009	1
Caelo	Macrogols 1500	17120011	2
Caelo	Macrogols 1500	17120012	3
Caelo	Macrogols 1500	18045703	1
Caelo	Macrogols 1500	1812905	1
Caelo	Macrogols 1500	18129503	1
Caelo	Macrogols 1500	18129505	1
Caelo	Macrogols 1500	18129506	1
Caelo	Macrogols 1500	18229002	2
Caelo	Macrogols 1500	18229004	2
Caelo	Macrogols 1500	192333501	1
Caelo	Macrogols 1500	19233501	3
Caelo	Macrogols 1500	20000729002	1
Caelo	Macrogols 1500	20000729005	1
Caesar & Loretz GmbH…	Macrogols 1500	21003420001	1
Caesar & Loretz GmbH	Macrogols 1500	19233501	1
Caesar & Loretz GmbH	Macrogols 1500	19233502	1
Caesar & Loretz GmbH	Macrogols 1500	20000729004	1
Caesar & Loretz GmbH	Macrogols 1500	21001042001	1
Caesar & Loretz GmbH	Macrogols 1500	21001042002	2
Caesar & Loretz GmbH	Macrogols 1500	21003420007	1
Euro OTC	Macrogols 1500	1103017-02	4
Euro OTC	Macrogols 1500	1206005-01	5
Euro OTC	Macrogols 1500	1304023-01	7
Euro OTC	Macrogols 1500	1406004-01	2
Euro OTC	Macrogols 1500	1503026-01	4
Euro OTC	Macrogols 1500	1806015-01	1
Euro OTC	Macrogols 1500	2009003-01	1
Gehe	Macrogols 1500	14072409	1
Krieger	Macrogols 1500	1712002	1
phoenix	Macrogols 1500	18229004	1
Phönix	Macrogols 1500	14072402	1

- 235 982 spectra from 1515 *Apo-Ident* customers from a total of 49 212 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Macrogols 1500* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Macrogols 1500* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	450	0	152 512
Type B	0	240	0	201 844
Type C	0	85	0	235 982

The substance/substance group *Macrogols 1500* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6667 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 92.9412 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20977	20977	0.00	65.25
21948	21948	0.00	88.41
22544	22544	0.00	117.62
23241	23291	10.88	56.72
23291	23291	0.00	57.01
25302	25302	0.00	68.17
25988	23291	6.41	54.98
27236	27236	0.00	91.78
27323	27323	0.00	68.89

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Macrogols 4000**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20690-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Macrogols 4000; Macrogolum 4000

Special notes

When selecting the *Macrogols 4000* substance/substance group, the following information is displayed to the user:

- Advice for the distinction from Macrogol 6000: Macrogol 4000 cannot be certainly distinct from Macrogol 6000, which is however currently not deliverable in Germany. Please decide, if an additional analysis seems reasonable.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Macrogols 4000	15	36	583

Second-stage model

For differentiation of the substance/substance group *Macrogols 4000* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Macrogols 4000* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Macrogols 1500	35.91	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Macrogols 4000* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Macrogols 4000*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Macrogols 4000	12074116	20690	40	1401164
Caelo	Macrogols 4000	12318019	20975	40	1403322
Caelo	Macrogols 4000	12361502	21065	40	20130107
Caelo	Macrogols 4000	13356616	21357	40	20131107
Euro OTC	Macrogols 4000	1507004	21841	60	0000010550
Euro OTC	Macrogols 4000	1508031	21903	60	20150914*
Euro OTC	Macrogols 4000	1605012	22567	40	20160606*
Euro OTC	Macrogols 4000	1605025	22570	40	20160603*
Euro OTC	Macrogols 4000	1702003	23174	40	20170301*
Euro OTC	Macrogols 4000	1711016	23902	40	20171214*
Euro OTC	Macrogols 4000	2009016	25414	40	20200928*
Euro OTC	Macrogols 4000	2104009	25713	50	20210624*
Euro OTC	Macrogols 4000	2207019	26262	40	20220728*
Euro OTC	Macrogols 4000	2207019	26262SI	20	20220728*
Fagron	Macrogols 4000	15B13-B04-305461	21886	60	AR-16-FG-004020-01
Fagron	Macrogols 4000	16F10-B04-325645	23021	40	20160822

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 690 spectra of 16 reference samples from the substance/substance group *Macrogols 4000*. These samples are listed above in the *calibration samples* section. The reference samples come from 15 different batches.

- 152 272 spectra from a total of 2827 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1490 spectra of 39 reference samples from the substance/substance group *Macrogols 4000*.

- Among them are spectra of independent samples from 36 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Macrogols 4000	11172433	20692	40
Caelo	Macrogols 4000	170686	23280	40
Caelo	Macrogols 4000	171190	23282	40
Caelo	Macrogols 4000	172081	23657	40
Caelo	Macrogols 4000	173039	23825	40
Caelo	Macrogols 4000	181974	24227	40
Caelo	Macrogols 4000	182154	24229	40
Caelo	Macrogols 4000	182448	24352	40
Caelo	Macrogols 4000	183153	24360	40
Caelo	Macrogols 4000	190093	24564	40
Caelo	Macrogols 4000	191756	24743	40
Caelo	Macrogols 4000	21001852005	26317	30
Caelo	Macrogols 4000	22003823	26477	40
Caelo	Macrogols 4000	22003814	26496	40
Caelo	Macrogols 4000	23000401	26691	40
Caelo	Macrogols 4000	24001280	27234	40
Caelo	Macrogols 4000	24002011	27445	40
Caelo	Macrogols 4000	24002115	27449	40
Euro OTC	Macrogols 4000	1609018	22791	40
Euro OTC	Macrogols 4000	1701007	22983	40
Euro OTC	Macrogols 4000	1705019	23433	40
Euro OTC	Macrogols 4000	1707026	23537	40
Euro OTC	Macrogols 4000	1804001	24089	40
Euro OTC	Macrogols 4000	1803029	24094	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Macrogols 4000	1810003	24339	40
Euro OTC	Macrogols 4000	1902009	24463	40
Euro OTC	Macrogols 4000	1907002	24798	40
Euro OTC	Macrogols 4000	1911027	25073	40
Euro OTC	Macrogols 4000	2007005	25326	40
Euro OTC	Macrogols 4000	2109002	25820	50
Euro OTC	Macrogols 4000	2207018	26276	40
Euro OTC	Macrogols 4000	2211018	26524	40
Euro OTC	Macrogols 4000	2401006	27153	40
Euro OTC	Macrogols 4000	2408012	27403	40
Fagron	Macrogols 4000	22A15-B06-216742	26071	40
Fagron	Macrogols 4000	24A19-B01-235824	27385	40
Caelo	Macrogols 4000	21001852005	26317SI	20
Euro OTC	Macrogols 4000	2207018	26276SI	20
Fagron	Macrogols 4000	22A15-B06-216742	26071SI	10

- 200 594 spectra from a total of 4009 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2313 spectra from 575 *Apo-Ident* customers from 591 batches from the substance/substance group *Macrogols 4000*.

- Among them are spectra of independent samples from 583 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Macrogols 4000	22001587006	1
	Macrogols 4000	22001929004	1
	Macrogols 4000	22003814008	1
	Macrogols 4000	22003814011	3
	Macrogols 4000	22003823005	6
	Macrogols 4000	22004211004	3
	Macrogols 4000	22004211006	2
	Macrogols 4000	22004211008	1
	Macrogols 4000	22004212003	4
	Macrogols 4000	22004213003	2
	Macrogols 4000	22004213004	3
	Macrogols 4000	22004213005	6
	Macrogols 4000	23001960006	1
	Macrogols 4000	23001960007	2
	Macrogols 4000	23001960008	7
	Macrogols 4000	23001960010	3
	Macrogols 4000	23002714002	2
	Macrogols 4000	23002714003	2
	Macrogols 4000	23002714004	2
	Macrogols 4000	23002741005	1
	Macrogols 4000	23C08-B02-228457	9
	Macrogols 4000	23C08-B02-229898	3
	Macrogols 4000	23C16-B18-229946	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Macrogols 4000	23C16-B18-229947	12
	Macrogols 4000	23C16-B18-2302203	1
	Macrogols 4000	23C16-B18-230223	1
	Macrogols 4000	24000623002	1
	Macrogols 4000	24000623006	1
	Macrogols 4000	24001280006	1
ACM	Macrogols 4000	KNC0366J15	2
AHC	Macrogols 4000	19000679007	1
AHC	Macrogols 4000	22004211001	1
AHD/Caesar & Loretz GmbH	Macrogols 4000	21001852005	1
AHD	Macrogols 4000	11H11-B05340782	1
AHD	Macrogols 4000	14L12-B06-301991	2
AHD	Macrogols 4000	15G15B07-313592	1
AHD	Macrogols 4000	16K25-B02-330527	3
AHD	Macrogols 4000	17208106	1
AHD	Macrogols 4000	17E02-B03	1
AHD	Macrogols 4000	17E02-B03-335507	3
AHD	Macrogols 4000	17K06-B05	2
AHD	Macrogols 4000	17K06-B05-345076	1
AHD	Macrogols 4000	18G30-B01	2
AHD	Macrogols 4000	18G30-B01-352394	2
AHD	Macrogols 4000	19000679005	1
AHD	Macrogols 4000	20001517005	1
AHD	Macrogols 4000	22004211006	1
AHD	Macrogols 4000	22004213005	1
AHD	Macrogols 4000	2211018-02	1
AHD	Macrogols 4000	23001960008	2
AHD	Macrogols 4000	23002714002	1
AHD	Macrogols 4000	23C16-B18-229946	1
AHD	Macrogols 4000	23C16-B18-229947	1
Alliance Healthcare	Macrogols 4000	12361512	2
Alliance	Macrogols 4000	18215403	1
Alliance	Macrogols 4000	20H21-F16-374090	1
Alliance	Macrogols 4000	21003792003	2
Alliance	Macrogols 4000	2109002-01	2
Alliance	Macrogols 4000	22001587010	3
Alliance	Macrogols 4000	22004211004	2
alliance	Macrogols 4000	23001960009	1
ANZAG 15.05.2014	Macrogols 4000	13356616	1
Anzag	Macrogols 4000	17068603	1
Audor Pharma	Macrogols 4000	2207018-01	2
Bombastus	Macrogols 4000	13136016	1
caedo	Macrogols 4000	17303902	2
Caelo	Macrogols 4000		1
Caelo	Macrogols 4000	1(20001517003)	1
Caelo	Macrogols 4000	1(20003397010)	1
Caelo	Macrogols 4000	1010023-02	1
Caelo	Macrogols 4000	1030517	1
Caelo	Macrogols 4000	11172303	1
Caelo	Macrogols 4000	1131117/16358107	1
Caelo	Macrogols 4000	1172404	1
Caelo	Macrogols 4000	1180513	1
Caelo	Macrogols 4000	1200617/16368105	1
Caelo	Macrogols 4000	12074102	1
Caelo	Macrogols 4000	12074109	3
Caelo	Macrogols 4000	12074114	1
Caelo	Macrogols 4000	12074116	3
Caelo	Macrogols 4000	12149108	1
Caelo	Macrogols 4000	12149113	2
Caelo	Macrogols 4000	12318011	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Macrogols 4000	12318019	1
Caelo	Macrogols 4000	12318027	1
Caelo	Macrogols 4000	1234	1
Caelo	Macrogols 4000	12345	1
Caelo	Macrogols 4000	1234Test	1
Caelo	Macrogols 4000	12361502	3
Caelo	Macrogols 4000	12361506	3
Caelo	Macrogols 4000	12361512	2
Caelo	Macrogols 4000	12361513	3
Caelo	Macrogols 4000	12361518	3
Caelo	Macrogols 4000	123test	1
Caelo	Macrogols 4000	123Test	1
Caelo	Macrogols 4000	1260917/16358105	1
Caelo	Macrogols 4000	13081501	1
Caelo	Macrogols 4000	13136001	3
Caelo	Macrogols 4000	13136003	3
Caelo	Macrogols 4000	13136009	3
Caelo	Macrogols 4000	13136010	1
Caelo	Macrogols 4000	13136011	4
Caelo	Macrogols 4000	1316003	1
Caelo	Macrogols 4000	13335102	1
Caelo	Macrogols 4000	13335106	1
Caelo	Macrogols 4000	13335107	1
Caelo	Macrogols 4000	13335120	1
Caelo	Macrogols 4000	13356601	4
Caelo	Macrogols 4000	13356602	3
Caelo	Macrogols 4000	13356609	1
Caelo	Macrogols 4000	13356611	4
Caelo	Macrogols 4000	13356616	1
Caelo	Macrogols 4000	13356617	6
Caelo	Macrogols 4000	13356621	1
Caelo	Macrogols 4000	1401708	1
Caelo	Macrogols 4000	14061705	5
Caelo	Macrogols 4000	14061707	4
Caelo	Macrogols 4000	14061708	9
Caelo	Macrogols 4000	14061713	1
Caelo	Macrogols 4000	14180503	1
Caelo	Macrogols 4000	14180504	1
Caelo	Macrogols 4000	14180508	2
Caelo	Macrogols 4000	14180511	2
Caelo	Macrogols 4000	14180520	4
Caelo	Macrogols 4000	14180522	1
Caelo	Macrogols 4000	14180524	1
Caelo	Macrogols 4000	14180525	3
Caelo	Macrogols 4000	14196007	1
Caelo	Macrogols 4000	14196013	1
Caelo	Macrogols 4000	14196017	1
Caelo	Macrogols 4000	143526	1
Caelo	Macrogols 4000	14352606	2
Caelo	Macrogols 4000	14352607	2
Caelo	Macrogols 4000	14352608	1
Caelo	Macrogols 4000	14352611	2
Caelo	Macrogols 4000	14352613	5
Caelo	Macrogols 4000	14352614	1
Caelo	Macrogols 4000	14352618	2
Caelo	Macrogols 4000	14J03-B07-304700	3
Caelo	Macrogols 4000	1508031-02	1
Caelo	Macrogols 4000	15159502	3
Caelo	Macrogols 4000	15159504	3
Caelo	Macrogols 4000	15159514	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Macrogols 4000	15159515	4
Caelo	Macrogols 4000	15159516	1
Caelo	Macrogols 4000	1517003	1
Caelo	Macrogols 4000	15225001	1
Caelo	Macrogols 4000	15225003	4
Caelo	Macrogols 4000	15225013	1
Caelo	Macrogols 4000	15335001	10
Caelo	Macrogols 4000	15335002	3
Caelo	Macrogols 4000	15335003	6
Caelo	Macrogols 4000	15335004	1
Caelo	Macrogols 4000	15335007	4
Caelo	Macrogols 4000	1535004	1
Caelo	Macrogols 4000	15376503	3
Caelo	Macrogols 4000	15376515	1
Caelo	Macrogols 4000	15376518	1
Caelo	Macrogols 4000	15376519	1
Caelo	Macrogols 4000	15406301	9
Caelo	Macrogols 4000	15406302	2
Caelo	Macrogols 4000	15406303	4
Caelo	Macrogols 4000	15406306	2
Caelo	Macrogols 4000	16023903	5
Caelo	Macrogols 4000	16023904	4
Caelo	Macrogols 4000	16023905	4
Caelo	Macrogols 4000	16023907	1
Caelo	Macrogols 4000	160912M	1
Caelo	Macrogols 4000	161017M/15406304	1
Caelo	Macrogols 4000	161202M/16152004	1
Caelo	Macrogols 4000	16152001	16
Caelo	Macrogols 4000	16152002	2
Caelo	Macrogols 4000	16152003	4
Caelo	Macrogols 4000	16267305	9
Caelo	Macrogols 4000	16267307	16
Caelo	Macrogols 4000	16267308	3
Caelo	Macrogols 4000	16267308/170227M	1
Caelo	Macrogols 4000	16267311	6
Caelo	Macrogols 4000	16308902	11
Caelo	Macrogols 4000	16308904	7
Caelo	Macrogols 4000	16308905	3
Caelo	Macrogols 4000	16308907	13
Caelo	Macrogols 4000	16308908	4
Caelo	Macrogols 4000	16358101	2
Caelo	Macrogols 4000	16358106	3
Caelo	Macrogols 4000	16358107	1
Caelo	Macrogols 4000	16358107/1111217	1
Caelo	Macrogols 4000	170105M16152004	1
Caelo	Macrogols 4000	170324M/16267308	1
Caelo	Macrogols 4000	17035603	2
Caelo	Macrogols 4000	17035604	4
Caelo	Macrogols 4000	17035606	13
Caelo	Macrogols 4000	17035607	5
Caelo	Macrogols 4000	17035608	1
Caelo	Macrogols 4000	170504M/16308906	1
Caelo	Macrogols 4000	170529M/16267308	1
Caelo	Macrogols 4000	170612M/17035603	1
Caelo	Macrogols 4000	17068603	4
Caelo	Macrogols 4000	170710M/17035603	1
Caelo	Macrogols 4000	170817M/17035603	1
Caelo	Macrogols 4000	170928M/17119002	1
Caelo	Macrogols 4000	171103M/17119002	1
Caelo	Macrogols 4000	17119001	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Macrogols 4000	17119005	2
Caelo	Macrogols 4000	171211M/17119003	1
Caelo	Macrogols 4000	17185601	2
Caelo	Macrogols 4000	1720103	1
Caelo	Macrogols 4000	17208103	13
Caelo	Macrogols 4000	17208104	24
Caelo	Macrogols 4000	17208105	2
Caelo	Macrogols 4000	17208106	2
Caelo	Macrogols 4000	1720813	1
Caelo	Macrogols 4000	17303901	18
Caelo	Macrogols 4000	17303902	9
Caelo	Macrogols 4000	17303903	1
Caelo	Macrogols 4000	17303905	1
Caelo	Macrogols 4000	17337901	6
Caelo	Macrogols 4000	17337902/1250418	1
Caelo	Macrogols 4000	17337902/1300518	1
Caelo	Macrogols 4000	17337902/2190218	1
Caelo	Macrogols 4000	17337906	1
Caelo	Macrogols 4000	177337906	1
Caelo	Macrogols 4000	18106101	2
Caelo	Macrogols 4000	18106103	5
Caelo	Macrogols 4000	18106104	6
Caelo	Macrogols 4000	18106105	34
Caelo	Macrogols 4000	18106106	9
Caelo	Macrogols 4000	18106109	5
Caelo	Macrogols 4000	18106110	4
Caelo	Macrogols 4000	18215403	4
Caelo	Macrogols 4000	18215404	5
Caelo	Macrogols 4000	18215405	2
Caelo	Macrogols 4000	18244802	18
Caelo	Macrogols 4000	18244803	11
Caelo	Macrogols 4000	18244805	14
Caelo	Macrogols 4000	18244806	4
Caelo	Macrogols 4000	18244809	2
Caelo	Macrogols 4000	18315301	17
Caelo	Macrogols 4000	18315302	11
Caelo	Macrogols 4000	18315303	13
Caelo	Macrogols 4000	18315304	6
Caelo	Macrogols 4000	18315305	8
Caelo	Macrogols 4000	18315307	20
Caelo	Macrogols 4000	18K01-B01-356808	1
Caelo	Macrogols 4000	190000679004	1
Caelo	Macrogols 4000	19000379004	1
Caelo	Macrogols 4000	1900067007	1
Caelo	Macrogols 4000	190006790006	1
Caelo	Macrogols 4000	19000679004	8
Caelo	Macrogols 4000	19000679005	10
Caelo	Macrogols 4000	19000679006	10
Caelo	Macrogols 4000	19000679007	24
Caelo	Macrogols 4000	19000679009	5
Caelo	Macrogols 4000	1900067909	1
Caelo	Macrogols 4000	1900679005	1
Caelo	Macrogols 4000	19009302	4
Caelo	Macrogols 4000	19009303	5
Caelo	Macrogols 4000	19009305	6
Caelo	Macrogols 4000	19009308	3
Caelo	Macrogols 4000	19009312	2
Caelo	Macrogols 4000	19009313	1
Caelo	Macrogols 4000	19009314	3
Caelo	Macrogols 4000	190908001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Macrogols 4000	19090801	1
Caelo	Macrogols 4000	19090804	1
Caelo	Macrogols 4000	190920	1
Caelo	Macrogols 4000	19142401	20
Caelo	Macrogols 4000	19142402	9
Caelo	Macrogols 4000	19142403	20
Caelo	Macrogols 4000	19142404	4
Caelo	Macrogols 4000	19142407	1
Caelo	Macrogols 4000	19175603	6
Caelo	Macrogols 4000	19175604	4
Caelo	Macrogols 4000	19175605	6
Caelo	Macrogols 4000	19175606	16
Caelo	Macrogols 4000	19175607	4
Caelo	Macrogols 4000	192227702	1
Caelo	Macrogols 4000	192277002	5
Caelo	Macrogols 4000	19227701	9
Caelo	Macrogols 4000	19227702	23
Caelo	Macrogols 4000	19227703	7
Caelo	Macrogols 4000	19227704	1
Caelo	Macrogols 4000	19227705	1
Caelo	Macrogols 4000	2(20003397010)	1
Caelo	Macrogols 4000	200002443005	1
Caelo	Macrogols 4000	200003397002	1
Caelo	Macrogols 4000	200003397005	1
Caelo	Macrogols 4000	200003397013	1
Caelo	Macrogols 4000	200003882003	1
Caelo	Macrogols 4000	20001303003	3
Caelo	Macrogols 4000	20001303007	1
Caelo	Macrogols 4000	2000151003	1
Caelo	Macrogols 4000	20001517001	1
Caelo	Macrogols 4000	20001517002	1
Caelo	Macrogols 4000	20001517003	24
Caelo	Macrogols 4000	20001517004	9
Caelo	Macrogols 4000	20001517005	8
Caelo	Macrogols 4000	20001517006	15
Caelo	Macrogols 4000	20001517008	1
Caelo	Macrogols 4000	20001517009	1
Caelo	Macrogols 4000	20002443003	2
Caelo	Macrogols 4000	20002443004	15
Caelo	Macrogols 4000	20002443005	7
Caelo	Macrogols 4000	20002443006	2
Caelo	Macrogols 4000	20002443007	11
Caelo	Macrogols 4000	20002443008	9
Caelo	Macrogols 4000	20002443009	7
Caelo	Macrogols 4000	20002443010	22
Caelo	Macrogols 4000	20002446004	1
Caelo	Macrogols 4000	20002494004	1
Caelo	Macrogols 4000	20003397002	26
Caelo	Macrogols 4000	20003397003	3
Caelo	Macrogols 4000	20003397004	14
Caelo	Macrogols 4000	20003397005	5
Caelo	Macrogols 4000	20003397007	15
Caelo	Macrogols 4000	20003397009	9
Caelo	Macrogols 4000	20003397010	13
Caelo	Macrogols 4000	20003397011	5
Caelo	Macrogols 4000	20003397012	7
Caelo	Macrogols 4000	20003397013	4
Caelo	Macrogols 4000	20003397014	7
Caelo	Macrogols 4000	20003397104	1
Caelo	Macrogols 4000	20003827001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Macrogols 4000	20003827006	4
Caelo	Macrogols 4000	20003827011	3
Caelo	Macrogols 4000	20003882001	4
Caelo	Macrogols 4000	20003882002	16
Caelo	Macrogols 4000	20003882003	5
Caelo	Macrogols 4000	20003882005	2
Caelo	Macrogols 4000	2000397004	1
Caelo	Macrogols 4000	2000397014	1
Caelo	Macrogols 4000	2001517003	1
Caelo	Macrogols 4000	2003397013	1
Caelo	Macrogols 4000	200691307	1
Caelo	Macrogols 4000	210003792002	1
Caelo	Macrogols 4000	21001520001	1
Caelo	Macrogols 4000	2100152006	1
Caelo	Macrogols 4000	21001845001	7
Caelo	Macrogols 4000	21001845002	5
Caelo	Macrogols 4000	21001846001	7
Caelo	Macrogols 4000	21001850001	1
Caelo	Macrogols 4000	21001850003	14
Caelo	Macrogols 4000	21001850005	6
Caelo	Macrogols 4000	21001850007	7
Caelo	Macrogols 4000	21001852005	13
Caelo	Macrogols 4000	21001852006	5
Caelo	Macrogols 4000	21001852007	6
Caelo	Macrogols 4000	21001852008	1
Caelo	Macrogols 4000	21003792002	11
Caelo	Macrogols 4000	21003792003	4
Caelo	Macrogols 4000	21003792004	6
Caelo	Macrogols 4000	21003792005	6
Caelo	Macrogols 4000	21003792006	1
Caelo	Macrogols 4000	21003795003	1
Caelo	Macrogols 4000	210037992003	1
Caelo	Macrogols 4000	210906(2101845001)	1
Caelo	Macrogols 4000	210923(20003397010)	1
Caelo	Macrogols 4000	211019(21001846001)	1
Caelo	Macrogols 4000	211124(21001850005)	1
Caelo	Macrogols 4000	211215(21001850005)	1
Caelo	Macrogols 4000	22001201001	1
Caelo	Macrogols 4000	22001587004	1
Caelo	Macrogols 4000	22001587005	9
Caelo	Macrogols 4000	22001587006	4
Caelo	Macrogols 4000	22001587007	17
Caelo	Macrogols 4000	22001587010	3
Caelo	Macrogols 4000	22001587013	1
Caelo	Macrogols 4000	22001587014	2
Caelo	Macrogols 4000	22001587015	1
Caelo	Macrogols 4000	22003814005	1
Caelo	Macrogols 4000	22003814006	4
Caelo	Macrogols 4000	22003814007	1
Caelo	Macrogols 4000	22003814008	1
Caelo	Macrogols 4000	22003814009	5
Caelo	Macrogols 4000	22003814011	1
Caelo	Macrogols 4000	22003814012	5
Caelo	Macrogols 4000	22003814013	1
Caelo	Macrogols 4000	22003814014	3
Caelo	Macrogols 4000	22003823005	1
Caelo	Macrogols 4000	2200421003	1
Caelo	Macrogols 4000	22004211001	2
Caelo	Macrogols 4000	22004211002	1
Caelo	Macrogols 4000	22004211006	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Macrogols 4000	22004213004	1
Caelo	Macrogols 4000	22004213005	1
Caelo	Macrogols 4000	220042163003	1
Caelo	Macrogols 4000	220117	1
Caelo	Macrogols 4000	220210(21001845001)	1
Caelo	Macrogols 4000	220210(21001852006)	1
Caelo	Macrogols 4000	220315(21003792002)	2
Caelo	Macrogols 4000	220412(21003792002)	1
Caelo	Macrogols 4000	220428(21003792002)	1
Caelo	Macrogols 4000	220516(21003792005)	1
Caelo	Macrogols 4000	220519(21003792005)	1
Caelo	Macrogols 4000	220804(22001587007)	1
Caelo	Macrogols 4000	220905(22001587014)	1
Caelo	Macrogols 4000	22A15-B06	1
Caelo	Macrogols 4000	23001960008	1
Caelo	Macrogols 4000	23001960009	1
Caelo	Macrogols 4000	23061505	1
Caelo	Macrogols 4000	24000623005	1
Caelo	Macrogols 4000	280913C	2
Caelo	Macrogols 4000	28111706	1
Caelo	Macrogols 4000	3(20003397010)	1
Caelo	Macrogols 4000	30041803	1
Caelo	Macrogols 4000	39393137	1
Caelo	Macrogols 4000	3940608	1
Caelo	Macrogols 4000	4123585	1
Caelo	Macrogols 4000	5041701	1
Caelo	Macrogols 4000	5406301	1
Caelo	Macrogols 4000	9061805	1
Caelo	Macrogols 4000	90908	1
Caelo	Macrogols 4000	IntCh217002	1
Caesar & Loretz GmbH...	Macrogols 4000	21003792003	3
Caesar & Loretz GmbH...	Macrogols 4000	22003814007	3
Caesar & Loretz GmbH...	Macrogols 4000	20001517003	1
Caesar & Loretz GmbH...	Macrogols 4000	18315307	1
Caesar & Loretz GmbH...	Macrogols 4000	19000679007	1
Caesar & Loretz GmbH...	Macrogols 4000	19175606	1
Caesar & Loretz GmbH...	Macrogols 4000	22003823005	1
Caesar & Loretz GmbH...	Macrogols 4000	18315307	1
Caesar & Loretz GmbH...	Macrogols 4000	19142401	1
Caesar & Loretz GmbH/ AHD	Macrogols 4000	19009302	1
Caesar & Loretz GmbH...	Macrogols 4000	19000679007	1
Caesar & Loretz GmbH...	Macrogols 4000	20003882002	1
Caesar & Loretz GmbH...	Macrogols 4000	21001845001	1
Caesar & Loretz GmbH...	Macrogols 4000	21001852005	1
Caesar & Loretz GmbH/AHD	Macrogols 4000	19009302	1
Caesar & Loretz GmbH/AHD	Macrogols 4000	20003397002	1
Caesar & Loretz GmbH/AHD	Macrogols 4000	20003397007	2
Caesar & Loretz GmbH/AHD	Macrogols 4000	20003397009	1
Caesar & Loretz GmbH/AHD	Macrogols 4000	22001587010	2
Caesar & Loretz GmbH/AHD	Macrogols 4000	22004211006	1
Caesar & Loretz GmbH...	Macrogols 4000	19000679005	3
Caesar & Loretz GmbH...	Macrogols 4000	19227703	2
Caesar & Loretz GmbH...	Macrogols 4000	20003397010	2
Caesar & Loretz GmbH...	Macrogols 4000	22001587014	1
Caesar & Loretz GmbH/E	Macrogols 4000	19000679007	1
Caesar & Loretz GmbH...	Macrogols 4000	20001517003	1
Caesar & Loretz GmbH...	Macrogols 4000	20003397002	1
Caesar & Loretz GmbH/Gehe	Macrogols 4000	18244802	1
Caesar & Loretz GmbH/GEHE	Macrogols 4000	19000679004	1
Caesar & Loretz GmbH/Gehe	Macrogols 4000	19142401	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Gehe	Macrogols 4000	20001303003	1
Caesar & Loretz GmbH/Gehe	Macrogols 4000	20001517003	1
Caesar & Loretz GmbH/Gehe	Macrogols 4000	20003397003	1
Caesar & Loretz GmbH/gehe	Macrogols 4000	20003882001	1
Caesar & Loretz GmbH/Gehe	Macrogols 4000	20003882005	2
Caesar & Loretz GmbH/Gehe	Macrogols 4000	21001845001	1
Caesar & Loretz GmbH/Gehe	Macrogols 4000	21003792005	1
Caesar & Loretz GmbH/Gehe	Macrogols 4000	21003795003	1
Caesar & Loretz GmbH/Gehe	Macrogols 4000	22001587004	1
Caesar & Loretz GmbH/Gehe	Macrogols 4000	22003814014	2
Caesar & Loretz GmbH...	Macrogols 4000	20003882001	2
Caesar & Loretz GmbH...	Macrogols 4000	20003882005	1
Caesar & Loretz GmbH...	Macrogols 4000	19000679004	1
Caesar & Loretz GmbH...	Macrogols 4000	20002443008	1
Caesar & Loretz GmbH...	Macrogols 4000	21001845001	2
Caesar & Loretz GmbH...	Macrogols 4000	21001852005	2
Caesar & Loretz GmbH...	Macrogols 4000	21003792002	1
Caesar & Loretz GmbH...	Macrogols 4000	22001587007	3
Caesar & Loretz GmbH...	Macrogols 4000	22004211006	1
Caesar & Loretz GmbH...	Macrogols 4000	22004213004	1
Caesar & Loretz GmbH...	Macrogols 4000	18315307	1
Caesar & Loretz GmbH...	Macrogols 4000	20003397012	1
Caesar & Loretz GmbH...	Macrogols 4000	21001846001	1
Caesar & Loretz GmbH...	Macrogols 4000	21001850005	2
Caesar & Loretz GmbH...	Macrogols 4000	21001852005	1
Caesar & Loretz GmbH/PH	Macrogols 4000	19000679007	1
Caesar & Loretz GmbH...	Macrogols 4000	20002443008	2
Caesar & Loretz GmbH/Phoe	Macrogols 4000	20003397011	1
Caesar & Loretz GmbH...	Macrogols 4000	19090804	2
Caesar & Loretz GmbH...	Macrogols 4000	20003397011	4
Caesar & Loretz GmbH...	Macrogols 4000	20003882005	1
Caesar & Loretz GmbH...	Macrogols 4000	22001587007	2
Caesar & Loretz GmbH...	Macrogols 4000	21001852006	2
Caesar & Loretz GmbH...	Macrogols 4000	21003792005	2
Caesar & Loretz GmbH...	Macrogols 4000	23001960008	3
Caesar & Loretz GmbH/Sana	Macrogols 4000	20002443010	1
Caesar & Loretz GmbH...	Macrogols 4000	18106105	1
Caesar & Loretz GmbH...	Macrogols 4000	20003397002	1
Caesar & Loretz GmbH...	Macrogols 4000	20003397012	2
Caesar & Loretz GmbH...	Macrogols 4000	22003814011	1
Caesar & Loretz GmbH	Macrogols 4000	14180520	1
Caesar & Loretz GmbH	Macrogols 4000	17337911	1
Caesar & Loretz GmbH	Macrogols 4000	18106105	2
Caesar & Loretz GmbH	Macrogols 4000	18244802	2
Caesar & Loretz GmbH	Macrogols 4000	18244803	1
Caesar & Loretz GmbH	Macrogols 4000	18244806	1
Caesar & Loretz GmbH	Macrogols 4000	18315301	2
Caesar & Loretz GmbH	Macrogols 4000	18315302	5
Caesar & Loretz GmbH	Macrogols 4000	18315303	3
Caesar & Loretz GmbH	Macrogols 4000	18315307	6
Caesar & Loretz GmbH	Macrogols 4000	19000679004	3
Caesar & Loretz GmbH	Macrogols 4000	19000679006	3
Caesar & Loretz GmbH	Macrogols 4000	19000679007	11
Caesar & Loretz GmbH	Macrogols 4000	19009302	3
Caesar & Loretz GmbH	Macrogols 4000	19009303	1
Caesar & Loretz GmbH	Macrogols 4000	19009305	2
Caesar & Loretz GmbH	Macrogols 4000	19009308	9
Caesar & Loretz GmbH	Macrogols 4000	19009313	2
Caesar & Loretz GmbH	Macrogols 4000	19142401	8
Caesar & Loretz GmbH	Macrogols 4000	19142402	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Macrogols 4000	19142407	4
Caesar & Loretz GmbH	Macrogols 4000	19175605	1
Caesar & Loretz GmbH	Macrogols 4000	19175606	9
Caesar & Loretz GmbH	Macrogols 4000	19175607	2
Caesar & Loretz GmbH	Macrogols 4000	192277002	1
Caesar & Loretz GmbH	Macrogols 4000	19227702	7
Caesar & Loretz GmbH	Macrogols 4000	19227703	1
Caesar & Loretz GmbH	Macrogols 4000	20001517003	7
Caesar & Loretz GmbH	Macrogols 4000	20001517006	1
Caesar & Loretz GmbH	Macrogols 4000	20001517009	1
Caesar & Loretz GmbH	Macrogols 4000	20002443005	2
Caesar & Loretz GmbH	Macrogols 4000	20002443007	1
Caesar & Loretz GmbH	Macrogols 4000	20002443008	2
Caesar & Loretz GmbH	Macrogols 4000	20002443010	4
Caesar & Loretz GmbH	Macrogols 4000	20002494004	1
Caesar & Loretz GmbH	Macrogols 4000	20003397002	9
Caesar & Loretz GmbH	Macrogols 4000	20003397003	2
Caesar & Loretz GmbH	Macrogols 4000	20003397004	1
Caesar & Loretz GmbH	Macrogols 4000	20003397007	6
Caesar & Loretz GmbH	Macrogols 4000	20003397010	1
Caesar & Loretz GmbH	Macrogols 4000	20003397012	4
Caesar & Loretz GmbH	Macrogols 4000	20003397013	6
Caesar & Loretz GmbH	Macrogols 4000	20003397014	8
Caesar & Loretz GmbH	Macrogols 4000	20003882001	1
Caesar & Loretz GmbH	Macrogols 4000	20003882002	1
Caesar & Loretz GmbH	Macrogols 4000	21001845002	1
Caesar & Loretz GmbH	Macrogols 4000	21001846001	5
Caesar & Loretz GmbH	Macrogols 4000	21001850005	1
Caesar & Loretz GmbH	Macrogols 4000	21001850007	2
Caesar & Loretz GmbH	Macrogols 4000	21001852005	1
Caesar & Loretz GmbH	Macrogols 4000	21001852006	4
Caesar & Loretz GmbH	Macrogols 4000	21001852007	3
Caesar & Loretz GmbH	Macrogols 4000	21001852008	1
Caesar & Loretz GmbH	Macrogols 4000	21003792002	7
Caesar & Loretz GmbH	Macrogols 4000	21003792004	5
Caesar & Loretz GmbH	Macrogols 4000	21003792005	9
Caesar & Loretz GmbH	Macrogols 4000	22001587004	2
Caesar & Loretz GmbH	Macrogols 4000	22001587005	4
Caesar & Loretz GmbH	Macrogols 4000	22001587006	4
Caesar & Loretz GmbH	Macrogols 4000	22001587007	3
Caesar & Loretz GmbH	Macrogols 4000	22003814007	1
Caesar & Loretz GmbH	Macrogols 4000	22003814008	2
Caesar & Loretz GmbH	Macrogols 4000	22003814009	2
Caesar & Loretz GmbH	Macrogols 4000	22003814011	2
Caesar & Loretz GmbH	Macrogols 4000	22003814013	2
Caesar & Loretz GmbH	Macrogols 4000	22003823005	1
Caesar & Loretz GmbH	Macrogols 4000	F16-3740901	1
Caesar & Loretz Hild…	Macrogols 4000	19000679007	1
Caesar&Loretz GmbH/ …	Macrogols 4000	17068603	1
Caesar&Loretz GmbH/Anzag	Macrogols 4000	14196017	1
Calo, Hilden/ Phönix	Macrogols 4000	19142401	1
calo	Macrogols 4000	17303902	1
Cealo / Anzag	Macrogols 4000	211020(21001846001)	1
Cealo / Anzag	Macrogols 4000	211115(21001846001)	1
Cealo / Anzag	Macrogols 4000	211217(21001850005)	1
Cealo/Anzag	Macrogols 4000	21001850005	1
Cealo/Gehe	Macrogols 4000	16023907	1
Cealo/Jenne	Macrogols 4000	220125(21001852006)	1
DIV GH	Macrogols 4000	13/12	1
EuRho	Macrogols 4000	1206009-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Macrogols 4000	1005011-01	1
Euro OTC	Macrogols 4000	1202040-02	2
Euro OTC	Macrogols 4000	130502002	1
Euro OTC	Macrogols 4000	1305020-02	4
Euro OTC	Macrogols 4000	140701001	1
Euro OTC	Macrogols 4000	1507004-01	1
Euro OTC	Macrogols 4000	1508031-01	1
Euro OTC	Macrogols 4000	1508031-02	1
Euro OTC	Macrogols 4000	15159515	1
Euro OTC	Macrogols 4000	1705019-01	1
Euro OTC	Macrogols 4000	1707026-01	1
Euro OTC	Macrogols 4000	1711016-01	1
Euro OTC	Macrogols 4000	17303905	1
Euro OTC	Macrogols 4000	1808003-01	4
Euro OTC	Macrogols 4000	1808003-02	5
Euro OTC	Macrogols 4000	180803-02	1
Euro OTC	Macrogols 4000	1810003-01	2
Euro OTC	Macrogols 4000	18315307	1
Euro OTC	Macrogols 4000	1902009-01	4
Euro OTC	Macrogols 4000	1911027-01	12
Euro OTC	Macrogols 4000	2007005-01	5
Euro OTC	Macrogols 4000	2009016-01	4
Euro OTC	Macrogols 4000	210400901	1
Euro OTC	Macrogols 4000	2104009-01	2
Euro OTC	Macrogols 4000	2109002-03	1
Euro OTC	Macrogols 4000	22/28	1
Euro OTC	Macrogols 4000	2207018-01	4
Euro OTC	Macrogols 4000	2211018-01	4
Facron	Macrogols 4000	7022014C	1
Fagron	Macrogols 4000	10022015A	1
Fagron	Macrogols 4000	10022015B	1
Fagron	Macrogols 4000	1112M-02103	1
Fagron	Macrogols 4000	123Test	1
Fagron	Macrogols 4000	12F13-N01	1
Fagron	Macrogols 4000	12F29-N01	2
Fagron	Macrogols 4000	12F29-NO1	1
Fagron	Macrogols 4000	12I20-n03	1
Fagron	Macrogols 4000	12L10-N06	2
Fagron	Macrogols 4000	13356608	1
Fagron	Macrogols 4000	13A10-N01	1
Fagron	Macrogols 4000	13B20N01	1
Fagron	Macrogols 4000	13B20-N01	2
Fagron	Macrogols 4000	13E22-N03	6
Fagron	Macrogols 4000	13F12N09	1
Fagron	Macrogols 4000	13F12-N09	1
Fagron	Macrogols 4000	13G19-N08	2
Fagron	Macrogols 4000	13G19-N14	1
Fagron	Macrogols 4000	13I17-N03	1
Fagron	Macrogols 4000	13I30-N03	1
Fagron	Macrogols 4000	13L30-B31	1
Fagron	Macrogols 4000	13l30-N03	1
Fagron	Macrogols 4000	14A03B01	1
Fagron	Macrogols 4000	14A03-B01-289602	3
Fagron	Macrogols 4000	14A03-B01-289605	1
Fagron	Macrogols 4000	14D14-B06	1
Fagron	Macrogols 4000	14D14-B06-293453	2
Fagron	Macrogols 4000	14G15-B07-295632	1
Fagron	Macrogols 4000	14G21-B04-296899	1
Fagron	Macrogols 4000	14J03-B07300840	1
Fagron	Macrogols 4000	14J03-B07-300840	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Macrogols 4000	14K03-_b07-300522	1
Fagron	Macrogols 4000	14K03-B07-300522	2
Fagron	Macrogols 4000	14L12-B06	1
Fagron	Macrogols 4000	15/29-B01-318038	2
Fagron	Macrogols 4000	15092014A	1
Fagron	Macrogols 4000	15376510	1
Fagron	Macrogols 4000	15A08-B03-302761	1
Fagron	Macrogols 4000	15A08B03302762	1
Fagron	Macrogols 4000	15A08-B03-302762	3
Fagron	Macrogols 4000	15b03-b08-304701	1
Fagron	Macrogols 4000	15B13-B04-305461	3
Fagron	Macrogols 4000	15G15-B07	1
Fagron	Macrogols 4000	15G15-B07-313592	2
Fagron	Macrogols 4000	15H10-B04-314037	2
Fagron	Macrogols 4000	15H10-B04-31407	1
Fagron	Macrogols 4000	15I29-B01-318038	1
Fagron	Macrogols 4000	160514a	1
Fagron	Macrogols 4000	16102013A	1
Fagron	Macrogols 4000	16152002	1
Fagron	Macrogols 4000	16A20-B15-320060	1
Fagron	Macrogols 4000	16a20-b15-320652	8
Fagron	Macrogols 4000	16A20-B15-320652	6
Fagron	Macrogols 4000	16F10-B04-324270	1
Fagron	Macrogols 4000	16K25-B02-330527	2
Fagron	Macrogols 4000	17012014A	1
Fagron	Macrogols 4000	17E02-B03-335507	1
Fagron	Macrogols 4000	17E02-B03-335526	3
Fagron	Macrogols 4000	17H11-B05-39499	1
Fagron	Macrogols 4000	17I11-B01-341774	2
Fagron	Macrogols 4000	17K06-B05-345076	3
Fagron	Macrogols 4000	17K06-B05345096	1
Fagron	Macrogols 4000	17K06-B05-345096	2
Fagron	Macrogols 4000	1803029-01	2
Fagron	Macrogols 4000	18082014C	1
Fagron	Macrogols 4000	18D10-B04-349676	1
Fagron	Macrogols 4000	18G30-B01	2
Fagron	Macrogols 4000	18G30-B01-345096	1
Fagron	Macrogols 4000	18K01-B01	1
Fagron	Macrogols 4000	18K01-B01-355299	1
Fagron	Macrogols 4000	19142403	1
Fagron	Macrogols 4000	19B06-B04	1
Fagron	Macrogols 4000	19B06-B04-359646	2
Fagron	Macrogols 4000	19B06-B04-359656	1
Fagron	Macrogols 4000	19G17-B03-363522	1
Fagron	Macrogols 4000	19H08-B03-364385	2
Fagron	Macrogols 4000	19H28-F07	1
Fagron	Macrogols 4000	19H28-F07-3643908	1
Fagron	Macrogols 4000	19H28-F07-364398	2
Fagron	Macrogols 4000	19H28-fo7-364388	1
Fagron	Macrogols 4000	19J28-F03	3
Fagron	Macrogols 4000	19J28-F03-366720	2
Fagron	Macrogols 4000	20/46	1
Fagron	Macrogols 4000	20002443007	1
Fagron	Macrogols 4000	20092014A	1
Fagron	Macrogols 4000	20122013C	1
Fagron	Macrogols 4000	2022015A	1
Fagron	Macrogols 4000	20803-F03-369765	1
Fagron	Macrogols 4000	20B03-F03	4
Fagron	Macrogols 4000	20B03-F03-369410	7
Fagron	Macrogols 4000	20B03-F03-369411	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Macrogols 4000	20B03-F03-369424	1
Fagron	Macrogols 4000	20B03-F03-369426	4
Fagron	Macrogols 4000	20B03-F03-369765	2
Fagron	Macrogols 4000	20E19-F01	1
Fagron	Macrogols 4000	20E19-F01-3718706	1
Fagron	Macrogols 4000	20E19-F01-371876	1
Fagron	Macrogols 4000	20E19-F01-371877	1
Fagron	Macrogols 4000	20-E19-F01-371877	1
Fagron	Macrogols 4000	20E19-F01-371878	1
Fagron	Macrogols 4000	20H21-F16	3
Fagron	Macrogols 4000	20H21-F16-374092	2
Fagron	Macrogols 4000	20H21-F16-374094	2
Fagron	Macrogols 4000	20K16-F05	2
Fagron	Macrogols 4000	20K16-F05-376031	3
Fagron	Macrogols 4000	20K16-F05-376034	1
Fagron	Macrogols 4000	21/37	2
Fagron	Macrogols 4000	21052015A	1
Fagron	Macrogols 4000	2122013a	1
Fagron	Macrogols 4000	2122013b	1
Fagron	Macrogols 4000	21B12-F03-377352	1
Fagron	Macrogols 4000	21B23-F01	2
Fagron	Macrogols 4000	21B23-F01-377361	2
Fagron	Macrogols 4000	21E8-B05-216626	1
Fagron	Macrogols 4000	21K08-B09-213154	1
Fagron	Macrogols 4000	22062015A	1
Fagron	Macrogols 4000	22122014A	1
Fagron	Macrogols 4000	2215I-02103	1
Fagron	Macrogols 4000	22A15_B06_216742	1
Fagron	Macrogols 4000	22A15-B06	1
Fagron	Macrogols 4000	22A15-B06-216677	2
Fagron	Macrogols 4000	22A15-B06-216742	2
Fagron	Macrogols 4000	22A15-B06-220791	5
Fagron	Macrogols 4000	22A25-B03-221082	3
Fagron	Macrogols 4000	22A25B03-221660	1
Fagron	Macrogols 4000	22A25-B03-221660	2
Fagron	Macrogols 4000	22A25-B03-224251	4
Fagron	Macrogols 4000	22G05-B01-221487	2
Fagron	Macrogols 4000	22G05-B01-223076	2
Fagron	Macrogols 4000	22G05-B01-224252	6
Fagron	Macrogols 4000	22L07-B02-225861	2
Fagron	Macrogols 4000	23C16-B18-229947	1
Fagron	Macrogols 4000	25082014A	1
Fagron	Macrogols 4000	25322-68-3	1
Fagron	Macrogols 4000	26052014A	1
Fagron	Macrogols 4000	26082013A	1
Fagron	Macrogols 4000	28052014B	1
Fagron	Macrogols 4000	2818A-02103	1
Fagron	Macrogols 4000	290714c	1
Fagron	Macrogols 4000	2OB03-F03	2
Fagron	Macrogols 4000	30092014B	1
Fagron	Macrogols 4000	3032014B	1
Fagron	Macrogols 4000	30B03	1
Fagron	Macrogols 4000	3114I-02103	1
Fagron	Macrogols 4000	3217M-02103	1
Fagron	Macrogols 4000	505201C	1
Fagron	Macrogols 4000	701014	1
Fagron	Macrogols 4000	701014-0006	3
Fagron	Macrogols 4000	701014-0014	1
Fagron	Macrogols 4000	8012015A	1
Fagron	Macrogols 4000	8062015B	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Macrogols 4000	8062015C	1
Fagron	Macrogols 4000	914I-02103	1
Fagron	Macrogols 4000	F03-3667200	1
Fagron	Macrogols 4000	F07-3643808	1
Fagron	Macrogols 4000	F16-3740901	1
Fiebig	Macrogols 4000	13356601	1
Fiebig	Macrogols 4000	14180506	1
Fiebig	Macrogols 4000	15159514	1
Fiebig	Macrogols 4000	16152001	1
Fiebig	Macrogols 4000	16308907	1
Fiebig	Macrogols 4000	17035607	1
Finteler Apotheke	Macrogols 4000	16308907	2
Finteler Apotheke	Macrogols 4000	17035607	1
Gatt-Koller	Macrogols 4000	1420/04152915	1
Gatt-Koller	Macrogols 4000	1420/04153415	1
Gatt-Koller	Macrogols 4000	1802391	1
Gatt-Koller	Macrogols 4000	1804126	1
Gatt-Koller	Macrogols 4000	2792/07153315	1
Gatt-Koller	Macrogols 4000	4643/01170417	2
Gehe / EuRho	Macrogols 4000	1803029-01	1
GEHE 06.05.2014	Macrogols 4000	13356608	2
Gehe	Macrogols 4000	14K03-B07-300522	1
Gehe	Macrogols 4000	15159514	3
Gehe	Macrogols 4000	16267307	1
Gehe	Macrogols 4000	16308907	1
Gehe	Macrogols 4000	17208104	1
GEHE	Macrogols 4000	18106109	1
Gehe	Macrogols 4000	19009303	1
Gehe	Macrogols 4000	19142401	1
Gehe	Macrogols 4000	19175607	1
Gehe	Macrogols 4000	20001517003	2
Gehe	Macrogols 4000	21003795003	1
gehe	Macrogols 4000	22004213005	1
Gepepharm/ Gehe	Macrogols 4000	1508031-02	1
Gutenberg-Apotheke	Macrogols 4000	13356609	1
Hedinger	Macrogols 4000	13G19-N08	1
Henry Lamotte Oils GMBH	Macrogols 4000	16267308/170127M	1
Henry Lamotte/AHD	Macrogols 4000	17303901	1
Henry Lamotte	Macrogols 4000	1213test	1
Kehr	Macrogols 4000	16308907	1
Kehr	Macrogols 4000	18106105	1
Kehr	Macrogols 4000	22003823005	1
KÖGL	Macrogols 4000	1900232	1
Macgol 4000	Macrogols 4000	16267308	2
Macgol 4000	Macrogols 4000	16F10-B04	1
Nachprüfung	Macrogols 4000	14A03-B01-289605	1
Nachtestung-Verlängerung	Macrogols 4000	17/17	1
Noveda	Macrogols 4000	18315307	1
Noweda	Macrogols 4000	12361502	2
Noweda	Macrogols 4000	12361512	1
Noweda	Macrogols 4000	13136003	1
Noweda	Macrogols 4000	17303902	1
Noweda	Macrogols 4000	17E02-B03-335526	1
Noweda	Macrogols 4000	18106109	2
Noweda	Macrogols 4000	18315303	1
Noweda	Macrogols 4000	19H08-B03-364385	1
Noweda	Macrogols 4000	20001517003	1
Noweda	Macrogols 4000	20003397004	3
Noweda	Macrogols 4000	20003397010	1
Noweda	Macrogols 4000	20003397013	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Macrogols 4000	21001850003	1
Noweda	Macrogols 4000	22001587007	3
Noweda	Macrogols 4000	22003814013	2
Noweda	Macrogols 4000	2200421001	1
Noweda	Macrogols 4000	22004211002	2
Noweda	Macrogols 4000	22004212003	3
Noweda	Macrogols 4000	22004213004	2
Noweda	Macrogols 4000	22A15B06216742	1
Noweda	Macrogols 4000	23001960009	1
Noweda	Macrogols 4000	2300196007	1
Noweda	Macrogols 4000	23C08-B02-227792	1
Phoenix	Macrogols 4000	12258901	1
Phoenix	Macrogols 4000	16023905	1
Phoenix	Macrogols 4000	18315307	2
Phoenix	Macrogols 4000	19175606	1
Phoenix	Macrogols 4000	20003397002	1
Phönix	Macrogols 4000	1202040-02	1
phönix	Macrogols 4000	1502031-02	1
phönix	Macrogols 4000	1535007	1
phönix	Macrogols 4000	15406302	1
phönix	Macrogols 4000	16023904	1
phönix	Macrogols 4000	1605012-01	1
phönix	Macrogols 4000	1701007-01	3
Phönix	Macrogols 4000	1707026-01	1
PHÖNIX	Macrogols 4000	19000679007	1
Phönix	Macrogols 4000	19142401	1
Phönix	Macrogols 4000	19142403	4
Phönix	Macrogols 4000	20002443004	1
Phönix	Macrogols 4000	20002443009	1
PHÖNIX	Macrogols 4000	20003397002	1
Phönix	Macrogols 4000	20003827011	1
Phönix	Macrogols 4000	23002714005	1
Rondell Apotheke	Macrogols 4000	16023905	1
Sanacorp	Macrogols 4000	14061707	1
Sanacorp	Macrogols 4000	15376520	1
Sanacorp	Macrogols 4000	17208104	1
Sanacorp	Macrogols 4000	17303901	1
Sanacorp	Macrogols 4000	18244802	1
Sanacorp	Macrogols 4000	19000679007	1
Sanacorp	Macrogols 4000	19142401	1
Sanacorp	Macrogols 4000	20002443004	1
Sanacorp	Macrogols 4000	20003397011	1
Sanacorp	Macrogols 4000	20003397014	1
Sanacorp	Macrogols 4000	21003792004	1
Sanacorp	Macrogols 4000	22003814013	1
Sanacorp	Macrogols 4000	22004213005	1
Sanacorp	Macrogols 4000	2204213005	1
Sanacorp	Macrogols 4000	2207019-03	1
Sanacorp	Macrogols 4000	24000623005	1
Sanacorp	Macrogols 4000	2707018-01	2
Sanacorp	Macrogols 4000	F03-3694101	1
VDL	Macrogols 4000	16308906	1
WE:Sanacorp 19.10.20…	Macrogols 4000	15406301	2

- 233 754 spectra from 1515 *Apo-Ident* customers from a total of 48 675 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Macrogols 4000* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Macrogols 4000* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	690	0	152 272
Type B	0	1490	0	200 414
Type C	0	2309	4	233 751

The substance/substance group *Macrogols 4000* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1304 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.5973 %)
Type C	100.0000 % (> 99.9009 %)	99.8271 % (> 99.6974 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20690	20690	0.00	63.01
20975	20975	0.00	81.90
21065	21886	13.58	66.73
21357	21886	7.20	60.51
21841	21841	0.00	70.13
21886	21886	0.00	58.23
21903	21903	0.00	75.67
22567	22567	0.00	59.17
22570	22570	0.00	72.95
23021	21886	6.86	63.67
23174	23174	0.00	74.90
23902	23902	0.00	78.71
25414	25414	0.00	77.29
25713	25713	0.00	78.33
26262	26262	0.00	76.70

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Mafenide acetate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	24055-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mafenide acetate; Mafenidum aceticum

Special notes

When selecting the *Mafenide acetate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Mafenide acetate	2	1	0

Second-stage model

For differentiation of the substance/substance group *Mafenide acetate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Mafenide acetate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Clioquinol	71.81	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Mafenide acetate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Mafenide acetate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Mafenide acetate	20K06-B04-211072	26070	40	20201229
Fagron	Mafenide acetate	22B02-B03-222844	27172	40	241107539

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Mafenide acetate*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

- 152 882 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 70 spectra of 3 reference samples from the substance/substance group *Mafenide acetate*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Mafenide acetate	15J20-B05-342526	24574	40
Fagron	Mafenide acetate	20K06-B04-211072	26070SI†	10
Fagron	Mafenide acetate	22B02-B03-222844	27172SI†	20

- 202 014 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Mafenide acetate*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Mafenide acetate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mafenide acetate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

	False positive	True positive	False negative	True negative
Type A	0	80	0	152 882
Type B	0	70	0	202 014
Type C	0	0	0	236 067

The substance/substance group *Mafenide acetate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 91.4286 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26070	27172	18.71	98.91
27172	27172	0.00	89.80

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Magnesium chloride hexahydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10006390-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Magnesium chloride hexahydrate; Magnesii chloridum hexahydricum

Special notes

When selecting the *Magnesium chloride hexahydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Magnesium chloride hexahydrate	3	1	68

Second-stage model

For differentiation of the substance/substance group *Magnesium chloride hexahydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Magnesium chloride hexahydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	86.19	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Magnesium chloride hexahydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Magnesium chloride hexahydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Magnesium chloride hexahydrate	1802023-01	24275	40	20180223
Euro OTC	Magnesium chloride hexahydrate	2107014	25790	50	20210812*
Euro OTC	Magnesium chloride hexahydrate	2307025	27085	40	20230810*
Euro OTC	Magnesium chloride hexahydrate	2307025	27085SI	20	20230810*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 150 spectra of 4 reference samples from the substance/substance group *Magnesium chloride hexahydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 812 spectra from a total of 2839 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 60 spectra of 2 reference samples from the substance/substance group *Magnesium chloride hexahydrate*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Magnesium chloride hexahydrate	24A22-B03-235953	27267	40
Fagron	Magnesium chloride hexahydrate	24A22-B03-235953	27267SI	20

- 202 024 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 139 spectra from 49 *Apo-Ident* customers from 72 batches from the substance/substance group *Magnesium chloride hexahydrate*.

- Among them are spectra of independent samples from 67 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Anzag	Magnesium chloride hexahydrate	120802501	1
Anzag	Magnesium chloride hexahydrate	1304003-01	1
Caelo	Magnesium chloride hexahydrate		1
Caelo	Magnesium chloride hexahydrate	1108024-01	1
Caelo	Magnesium chloride hexahydrate	11345606	1
Caelo	Magnesium chloride hexahydrate	11345609	1
Caelo	Magnesium chloride hexahydrate	11345623	2
Caelo	Magnesium chloride hexahydrate	11345624	1
Caelo	Magnesium chloride hexahydrate	12141803	1
Caelo	Magnesium chloride hexahydrate	12141806	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Magnesium chloride hexahydrate	12141807	3
Caelo	Magnesium chloride hexahydrate	12141808	1
Caelo	Magnesium chloride hexahydrate	12141811	2
Caelo	Magnesium chloride hexahydrate	12141814	1
Caelo	Magnesium chloride hexahydrate	12141817	2
Caelo	Magnesium chloride hexahydrate	12354604	4
Caelo	Magnesium chloride hexahydrate	12354605	4
Caelo	Magnesium chloride hexahydrate	12354606	4
Caelo	Magnesium chloride hexahydrate	12354608	1
Caelo	Magnesium chloride hexahydrate	12354609	7
Caelo	Magnesium chloride hexahydrate	12354610	2
Caelo	Magnesium chloride hexahydrate	12354612	7
Caelo	Magnesium chloride hexahydrate	12354613	4
Caelo	Magnesium chloride hexahydrate	12354615	8
Caelo	Magnesium chloride hexahydrate	12354618	2
Caelo	Magnesium chloride hexahydrate	1304C004	1
Caelo	Magnesium chloride hexahydrate	13194701	1
Caelo	Magnesium chloride hexahydrate	13194702	3
Caelo	Magnesium chloride hexahydrate	13194706	3
Caelo	Magnesium chloride hexahydrate	13194707	4
Caelo	Magnesium chloride hexahydrate	13194713	1
Caelo	Magnesium chloride hexahydrate	13194713-3490312103	1
Caelo	Magnesium chloride hexahydrate	13194721	2
Caelo	Magnesium chloride hexahydrate	1512I-01828	1
Caelo	Magnesium chloride hexahydrate	16094004	1
Caelo	Magnesium chloride hexahydrate	16094014	1
Caelo	Magnesium chloride hexahydrate	17034304	1
Caelo	Magnesium chloride hexahydrate	5210I-01828	1
Caesar & Loretz GmbH	Magnesium chloride hexahydrate	13064223	1
Cealo	Magnesium chloride hexahydrate	112354615	1
Cealo	Magnesium chloride hexahydrate	11354615	1
Euro OTC	Magnesium chloride hexahydrate	1112013-01	2
Euro OTC	Magnesium chloride hexahydrate	1204017-01	1
Euro OTC	Magnesium chloride hexahydrate	1208025-01	1
Euro OTC	Magnesium chloride hexahydrate	1212013-01	3
Euro OTC	Magnesium chloride hexahydrate	1304003-01	1
Fagron	Magnesium chloride hexahydrate	11K17-N10	1
Fagron	Magnesium chloride hexahydrate	12B16-N01	1
Fagron	Magnesium chloride hexahydrate	12D11-N01	1
Fagron	Magnesium chloride hexahydrate	12h21-N02	1
Fagron	Magnesium chloride hexahydrate	12H21-N02	5
Fagron	Magnesium chloride hexahydrate	12H21-No2	1
Fagron	Magnesium chloride hexahydrate	12H21-NO2	1
Fagron	Magnesium chloride hexahydrate	1301c009-277802	1
Fagron	Magnesium chloride hexahydrate	1301C009-277802	4
Fagron	Magnesium chloride hexahydrate	1301C011-277803	1
Fagron	Magnesium chloride hexahydrate	1301C012-277804	1
Fagron	Magnesium chloride hexahydrate	1301C10	3
Fagron	Magnesium chloride hexahydrate	1301C10-277801	1
Fagron	Magnesium chloride hexahydrate	1304C001-281211	2
Fagron	Magnesium chloride hexahydrate	1304C002	1
Fagron	Magnesium chloride hexahydrate	1304C003	1
Fagron	Magnesium chloride hexahydrate	1304C003-281209	1
Fagron	Magnesium chloride hexahydrate	1304C004	1
Fagron	Magnesium chloride hexahydrate	1304c004-281210	1
Fagron	Magnesium chloride hexahydrate	1304C004-281210	1
Fagron	Magnesium chloride hexahydrate	13411207	1
Fagron	Magnesium chloride hexahydrate	13B14-B01-287292	1
Fagron	Magnesium chloride hexahydrate	26061305	1
Fagron	Magnesium chloride hexahydrate	M1430	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Magnesium chloride hexahydrate	M1555	1
Fagron	Magnesium chloride hexahydrate	M1625	1
Fragon/Sanacorp	Magnesium chloride hexahydrate	12H21-N02	4
Phönix/Euro	Magnesium chloride hexahydrate	1208025-01	1
stumpf	Magnesium chloride hexahydrate	1301c012-277804	1
unbekannt	Magnesium chloride hexahydrate	unbekannt	1

- 235 928 spectra from 1515 *Apo-Ident* customers from a total of 49 187 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Magnesium chloride hexahydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Magnesium chloride hexahydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	150	0	152 812
Type B	0	60	0	202 024
Type C	0	108	31	235 928

The substance/substance group *Magnesium chloride hexahydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.9007 %)	77.6978 % (> 75.5396 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24275	27085	21.08	152.02
25790	25790	0.00	159.37
27085	27085	0.00	155.46

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Magnesium citrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20616-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Magnesium citrate; Magnesii citras

Special notes

When selecting the *Magnesium citrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Magnesium citrate	13	6	18

Second-stage model

For differentiation of the substance/substance group *Magnesium citrate* the following second-stage model is used:

- Submodel 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Magnesium citrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	39.04	39.20
Polymyxin B sulfate	40.69	–
Sodium cromoglicate	63.43	–
⋮	⋮	⋮
Carbomers	66.36	63.43
Gentamicin sulfate	>50	103.36
Zinc gluconate	>50	147.96
Sodium tetraborate	>50	156.36
Mg-Ca-K colamine phosphate	>50	170.28
Tobramycin sulfate	>50	202.41
Neomycin sulfate	>50	215.38
Finasteride	>50	940.06

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Magnesium citrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Magnesium citrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Magnesium citrate	1501031	21794	60	AR-15-FG-007845-01
Euro OTC	Magnesium citrate	1506020	21829	60	20150623*
Euro OTC	Magnesium citrate	1507019	21860	60	20150722*
Euro OTC	Magnesium citrate	1511018	22225	60	20151130*
Euro OTC	Magnesium citrate	1602028	22505	40	20160314*
Euro OTC	Magnesium citrate	1706007	23549	40	20170720*
Euro OTC	Magnesium citrate	1711018	23895	40	20171129*
Euro OTC	Magnesium citrate	1803033	24088	40	20180403*
Euro OTC	Magnesium citrate	1808020	24202	40	20180827*
Euro OTC	Magnesium citrate	1902006	24480	40	20190226*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Magnesium citrate	2003051	25170	40	20200428*
Euro OTC	Magnesium citrate	2012001	25465	40	20201216*
Euro OTC	Magnesium citrate	2105003	25708	50	20210701*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 610 spectra of 13 reference samples from the substance/substance group *Magnesium citrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 13 different batches.

- 152 352 spectra from a total of 2829 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 280 spectra of 8 reference samples from the substance/substance group *Magnesium citrate*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Magnesium citrate	1607006	22673	40
Euro OTC	Magnesium citrate	1701018	22998	40
Euro OTC	Magnesium citrate	1810026	24308	40
Euro OTC	Magnesium citrate	1907040	24778	40
Euro OTC	Magnesium citrate	2212004	26530	40
Euro OTC	Magnesium citrate	2404010	27210	40
Euro OTC	Magnesium citrate	2212004	26530SI	20
Euro OTC	Magnesium citrate	2404010	27210SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 804 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 32 spectra from 25 *Apo-Ident* customers from 18 batches from the substance/substance group *Magnesium citrate*.
- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Magnesium citrate	2105003-01	1
	Magnesium citrate	2401010-01	1
AHD	Magnesium citrate	2212004-01	1
APOrtha Deutschland GmbH	Magnesium citrate	17000809/0	1
Arktis	Magnesium citrate	894P/2418	1
Caelo	Magnesium citrate	1701018-01	1
Euro OTC	Magnesium citrate	1602028-01	1
Euro OTC	Magnesium citrate	1706007-01	3
Euro OTC	Magnesium citrate	1711018-01	2
Euro OTC	Magnesium citrate	1808020-01	2
Euro OTC	Magnesium citrate	180820-01	1
Euro OTC	Magnesium citrate	1810026-01	2
Euro OTC	Magnesium citrate	1902006-01	3
Euro OTC	Magnesium citrate	1907040-01	4
Euro OTC	Magnesium citrate	2003051-01	3
Euro OTC	Magnesium citrate	2012001-01	1
Euro OTC	Magnesium citrate	2105003-01	1
Euro OTC	Magnesium citrate	3060884	2
Euro OTC	Magnesium citrate	3086441	1

- 236 035 spectra from 1515 *Apo-Ident* customers from a total of 49 240 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Magnesium citrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Magnesium citrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	610	0	152 352
Type B	0	280	0	201 804
Type C	0	32	0	236 035

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The substance/substance group *Magnesium citrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0164 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.8571 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 81.2500 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21794	21794	0.00	60.63
21829	21829	0.00	99.18
21860	21860	0.00	88.96
22225	22225	0.00	77.32
22505	22505	0.00	83.94
23549	23549	0.00	46.66
23895	23895	0.00	86.90
24088	24088	0.00	98.75
24202	24202	0.00	111.16
24480	24480	0.00	59.03
25170	25170	0.00	60.95
25465	25465	0.00	55.37
25708	25708	0.00	48.63

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Magnesium hydrogen aspartate tetrahydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20812-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Magnesium hydrogen aspartate tetrahydrate; Magnesii aspartas tetrahydricus

Special notes

When selecting the *Magnesium hydrogen aspartate tetrahydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Magnesium hydrogen aspartate tetrahydrate	7	6	10

Second-stage model

For differentiation of the substance/substance group *Magnesium hydrogen aspartate tetrahydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Magnesium hydrogen aspartate tetrahydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	73.96	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Magnesium hydrogen aspartate tetrahydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Magnesium hydrogen aspartate tetrahydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Magnesium hydrogen aspart…	1204014-01	20812	40	1404588
Euro OTC	Magnesium hydrogen aspart…	1306045-01	21749	60	20130708
Euro OTC	Magnesium hydrogen aspart…	1605031	22682	40	20160617*
Euro OTC	Magnesium hydrogen aspart…	1901036	24488	40	20190227*
Euro OTC	Magnesium hydrogen aspart…	1906029	24773	40	20190712*
Euro OTC	Magnesium hydrogen aspart…	2002039	25125	40	20200331*
Euro OTC	Magnesium hydrogen aspart…	2303004	26645	40	20230315*
Euro OTC	Magnesium hydrogen aspart…	2303004	26645SI	20	20230315*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 320 spectra of 8 reference samples from the substance/substance group *Magnesium hydrogen aspartate tetrahydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 642 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 320 spectra of 9 reference samples from the substance/substance group *Magnesium hydrogen aspartate tetrahydrate*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Magnesium hydrogen aspart…	1707010	23552	40
Euro OTC	Magnesium hydrogen aspart…	1806011	24156	40
Euro OTC	Magnesium hydrogen aspart…	2007041	25344	40
Euro OTC	Magnesium hydrogen aspart…	2101039	25737	40
Euro OTC	Magnesium hydrogen aspart…	2207024	26273	40
Euro OTC	Magnesium hydrogen aspart…	2407011	27340	40
Euro OTC	Magnesium hydrogen aspart…	1707010	23608	40
Euro OTC	Magnesium hydrogen aspart…	2207024	26273SI	20
Euro OTC	Magnesium hydrogen aspart…	2407011	27340SI	20

- 201 764 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 18 spectra from 4 *Apo-Ident* customers from 10 batches from the substance/substance group *Magnesium hydrogen aspartate tetrahydrate*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Magnesium hydrogen aspart…	2303004-01	1
Euro OTC	Magnesium hydrogen aspart…	1605031-01	1
Euro OTC	Magnesium hydrogen aspart…	1806011-01	1
Euro OTC	Magnesium hydrogen aspart…	1901036-02	1
Euro OTC	Magnesium hydrogen aspart…	2002039-01	3
Euro OTC	Magnesium hydrogen aspart…	2007041-01	3
Euro OTC	Magnesium hydrogen aspart…	210039-01	1
Euro OTC	Magnesium hydrogen aspart…	2101039-01	5
Euro OTC	Magnesium hydrogen aspart…	3068139	1
Euro OTC	Magnesium hydrogen aspart…	3843631-1	1

- 236 049 spectra from 1515 *Apo-Ident* customers from a total of 49 248 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Magnesium hydrogen aspartate tetrahydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Magnesium hydrogen aspartate tetrahydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	320	0	201 764
Type C	0	18	0	236 049

The substance/substance group *Magnesium hydrogen aspartate tetrahydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.1250 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20812	20812	0.00	147.41
21749	20812	11.69	149.05
22682	22682	0.00	145.28
24488	24488	0.00	145.18
24773	24773	0.00	146.10
25125	25125	0.00	149.66
26645	26645	0.00	149.70

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Magnesium hydrogen citrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20016-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Magnesium hydrogen citrate; Magnesii hydrogenocitras hydricus; Magnesium hydrogen citrate, hydrated

Special notes

When selecting the *Magnesium hydrogen citrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Magnesium hydrogen citrate	11	34	251

Second-stage model

For differentiation of the substance/substance group *Magnesium hydrogen citrate* the following second-stage model is used:

- Submodel 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Magnesium hydrogen citrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	48.65	–
Riboflavin sodium phosphate hydrate	62.79	–
⋮	⋮	⋮
Atropine sulfate	>50	76.24
Escin, water-soluble	>50	92.51
Mometasone furoate	>50	124.80
Calcium orotate dihydrate	>50	157.33
Quinoline yellow	>50	161.83
Saccharin sodium	>50	177.51
Hydrocortisone	>50	198.83
Propranolol hydrochloride	>50	319.89
Potassium sorbate	>50	479.19
Phenytoin	>50	584.28

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Magnesium hydrogen citrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Magnesium hydrogen citrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Magnesium hydrogen citrate	13389102	21445	60	20131205
Caelo	Magnesium hydrogen citrate	15415014	23240	40	20160105
Caelo	Magnesium hydrogen citrate	22001882	26251	40	2211127
Euro OTC	Magnesium hydrogen citrate	1507010	21873	60	20150713*
Euro OTC	Magnesium hydrogen citrate	1510033	22233	60	20151117*
Euro OTC	Magnesium hydrogen citrate	1601005	22296	60	20160119*
Euro OTC	Magnesium hydrogen citrate	1701003	22992	40	20170124*
Euro OTC	Magnesium hydrogen citrate	2101004	25545	40	20210114*
Euro OTC	Magnesium hydrogen citrate	2211017	26423	40	20221213*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Gatt-Koller	Magnesium hydrogen citrate	22J01469	26400	40	2301186
Gatt-Koller	Magnesium hydrogen citrate	22J01469	26400SI	20	2301186
Gatt-Koller	Magnesium hydrogen citrate	24J00867	27302	40	20240620

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 540 spectra of 12 reference samples from the substance/substance group *Magnesium hydrogen citrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 422 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1490 spectra of 40 reference samples from the substance/substance group *Magnesium hydrogen citrate*.

- Among them are spectra of independent samples from 34 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Magnesium hydrogen citrate	173531	23788	40
Caelo	Magnesium hydrogen citrate	182746	24397	40
Caelo	Magnesium hydrogen citrate	21000135	25694	50
Caelo	Magnesium hydrogen citrate	23001929	26956	40
Caelo	Magnesium hydrogen citrate	24000609	27126	40
Caelo	Magnesium hydrogen citrate	24001460	27305	40
Euro OTC	Magnesium hydrogen citrate	1604002	22509	40
Euro OTC	Magnesium hydrogen citrate	1608004	22796	40
Euro OTC	Magnesium hydrogen citrate	1701004	22991	40
Euro OTC	Magnesium hydrogen citrate	1705010	23380	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Magnesium hydrogen citrate	1705009	23382	40
Euro OTC	Magnesium hydrogen citrate	1710007	23771	40
Euro OTC	Magnesium hydrogen citrate	1802026	24064	40
Euro OTC	Magnesium hydrogen citrate	1811038	24425	40
Euro OTC	Magnesium hydrogen citrate	1904011	24620	40
Euro OTC	Magnesium hydrogen citrate	1907020	24777	40
Euro OTC	Magnesium hydrogen citrate	1910005	24934	40
Euro OTC	Magnesium hydrogen citrate	2003064	25261	40
Euro OTC	Magnesium hydrogen citrate	2005027	25281	40
Euro OTC	Magnesium hydrogen citrate	2009007	25329	40
Euro OTC	Magnesium hydrogen citrate	2104021	25679	40
Euro OTC	Magnesium hydrogen citrate	2107008	25777	50
Euro OTC	Magnesium hydrogen citrate	2110009	25871	50
Euro OTC	Magnesium hydrogen citrate	2201004	25918	40
Euro OTC	Magnesium hydrogen citrate	2206017	26202	40
Euro OTC	Magnesium hydrogen citrate	2304016	26644	40
Euro OTC	Magnesium hydrogen citrate	2303006	26648	40
Euro OTC	Magnesium hydrogen citrate	2307001	26878	40
Euro OTC	Magnesium hydrogen citrate	2310019	26999	40
Euro OTC	Magnesium hydrogen citrate	2403003	27195	40
Euro OTC	Magnesium hydrogen citrate	2407003	27348	40
Fagron	Magnesium hydrogen citrate	19I23-B02-195296	24953	40
Fagron	Magnesium hydrogen citrate	22F02-B17-221504	26170	40
Gatt-Koller	Magnesium hydrogen citrate	22J00225	26399	40
Caelo	Magnesium hydrogen citrate	22001882	26251SI[†]	20
Euro OTC	Magnesium hydrogen citrate	2110009	25871SI	10
Euro OTC	Magnesium hydrogen citrate	2201004	25918SI	10
Euro OTC	Magnesium hydrogen citrate	2206017	26202SI	20
Fagron	Magnesium hydrogen citrate	22F02-B17-221504	26170SI	20
Gatt-Koller	Magnesium hydrogen citrate	22J00225	26399SI	20

- 200 594 spectra from a total of 4010 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 811 spectra from 282 *Apo-Ident* customers from 256 batches from the substance/substance group *Magnesium hydrogen citrate*.

- Among them are spectra of independent samples from 249 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Magnesium hydrogen citrate	1311003-01	1
	Magnesium hydrogen citrate	1510033-01	1
	Magnesium hydrogen citrate	22001882002	1
	Magnesium hydrogen citrate	22001882003	1
	Magnesium hydrogen citrate	22002876002	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Magnesium hydrogen citrate	23001929001	1
	Magnesium hydrogen citrate	23002924003	1
	Magnesium hydrogen citrate	2304016-01	1
	Magnesium hydrogen citrate	24001460001	1
/Sanacorp	Magnesium hydrogen citrate	90170	1
ACM	Magnesium hydrogen citrate	KNC0829J15	1
ACM	Magnesium hydrogen citrate	KNC1377J15	2
AHD	Magnesium hydrogen citrate	13389103	1
Alliance health	Magnesium hydrogen citrate	13389111	2
Alliance	Magnesium hydrogen citrate	181103801	1
Anzag	Magnesium hydrogen citrate	16341710	1
AppliChem	Magnesium hydrogen citrate	7V008966	1
Bombastus	Magnesium hydrogen citrate	1608004-01	1
Caelo	Magnesium hydrogen citrate		1
Caelo	Magnesium hydrogen citrate	1014E-01829	1
Caelo	Magnesium hydrogen citrate	11021401	1
Caelo	Magnesium hydrogen citrate	11044103	2
Caelo	Magnesium hydrogen citrate	11061403	1
Caelo	Magnesium hydrogen citrate	11193104	1
Caelo	Magnesium hydrogen citrate	1119I-01829	1
Caelo	Magnesium hydrogen citrate	11372901	1
Caelo	Magnesium hydrogen citrate	11372902	1
Caelo	Magnesium hydrogen citrate	12091303	1
Caelo	Magnesium hydrogen citrate	121033-01	1
Caelo	Magnesium hydrogen citrate	1214	1
Caelo	Magnesium hydrogen citrate	12175801	1
Caelo	Magnesium hydrogen citrate	12175802	2
Caelo	Magnesium hydrogen citrate	12175807	3
Caelo	Magnesium hydrogen citrate	12175810	4
Caelo	Magnesium hydrogen citrate	12238002	3
Caelo	Magnesium hydrogen citrate	12238004	3
Caelo	Magnesium hydrogen citrate	12238012	1
Caelo	Magnesium hydrogen citrate	12368002	3
Caelo	Magnesium hydrogen citrate	12368003	9
Caelo	Magnesium hydrogen citrate	12368004	2
Caelo	Magnesium hydrogen citrate	12368005	1
Caelo	Magnesium hydrogen citrate	12368011	8
Caelo	Magnesium hydrogen citrate	12368014	2
Caelo	Magnesium hydrogen citrate	12368017	2
Caelo	Magnesium hydrogen citrate	13194601	4
Caelo	Magnesium hydrogen citrate	13194603	1
Caelo	Magnesium hydrogen citrate	13233901	9
Caelo	Magnesium hydrogen citrate	13233904	5
Caelo	Magnesium hydrogen citrate	13233905	1
Caelo	Magnesium hydrogen citrate	13233906	9
Caelo	Magnesium hydrogen citrate	13233907	2
Caelo	Magnesium hydrogen citrate	13233910	5
Caelo	Magnesium hydrogen citrate	13233911	3
Caelo	Magnesium hydrogen citrate	13233913	6
Caelo	Magnesium hydrogen citrate	133233907	1
Caelo	Magnesium hydrogen citrate	133389111	1
Caelo	Magnesium hydrogen citrate	13389103	7
Caelo	Magnesium hydrogen citrate	13389106	2
Caelo	Magnesium hydrogen citrate	13389107	2
Caelo	Magnesium hydrogen citrate	13389108	1
Caelo	Magnesium hydrogen citrate	13389111	4
Caelo	Magnesium hydrogen citrate	1415013	1
Caelo	Magnesium hydrogen citrate	14265503	6
Caelo	Magnesium hydrogen citrate	14265504	5
Caelo	Magnesium hydrogen citrate	14265505	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Magnesium hydrogen citrate	14265511	1
Caelo	Magnesium hydrogen citrate	14265513	2
Caelo	Magnesium hydrogen citrate	14265514	1
Caelo	Magnesium hydrogen citrate	14265516	3
Caelo	Magnesium hydrogen citrate	14265517	1
Caelo	Magnesium hydrogen citrate	14265520	1
Caelo	Magnesium hydrogen citrate	14265521	1
Caelo	Magnesium hydrogen citrate	14I12-B02-298854	1
Caelo	Magnesium hydrogen citrate	1507010-01	2
Caelo	Magnesium hydrogen citrate	15296701	10
Caelo	Magnesium hydrogen citrate	15296702	4
Caelo	Magnesium hydrogen citrate	15296709	6
Caelo	Magnesium hydrogen citrate	15296710	1
Caelo	Magnesium hydrogen citrate	15296712	2
Caelo	Magnesium hydrogen citrate	15296801	3
Caelo	Magnesium hydrogen citrate	15415001	6
Caelo	Magnesium hydrogen citrate	15415002	1
Caelo	Magnesium hydrogen citrate	15415003	6
Caelo	Magnesium hydrogen citrate	15415004	2
Caelo	Magnesium hydrogen citrate	15415005	3
Caelo	Magnesium hydrogen citrate	15415009	6
Caelo	Magnesium hydrogen citrate	15415010	9
Caelo	Magnesium hydrogen citrate	15415013	2
Caelo	Magnesium hydrogen citrate	15415014	6
Caelo	Magnesium hydrogen citrate	15415015	1
Caelo	Magnesium hydrogen citrate	160100501	1
Caelo	Magnesium hydrogen citrate	1601005-01	1
Caelo	Magnesium hydrogen citrate	1604002-01	3
Caelo	Magnesium hydrogen citrate	16341707	2
Caelo	Magnesium hydrogen citrate	16341708	5
Caelo	Magnesium hydrogen citrate	16341709	3
Caelo	Magnesium hydrogen citrate	16341710	6
Caelo	Magnesium hydrogen citrate	16341711	2
Caelo	Magnesium hydrogen citrate	16E02-B03-321485	1
Caelo	Magnesium hydrogen citrate	17061401	1
Caelo	Magnesium hydrogen citrate	1710007-01	2
Caelo	Magnesium hydrogen citrate	17173401	7
Caelo	Magnesium hydrogen citrate	17173404	1
Caelo	Magnesium hydrogen citrate	17173405	6
Caelo	Magnesium hydrogen citrate	17173406	3
Caelo	Magnesium hydrogen citrate	17173407	2
Caelo	Magnesium hydrogen citrate	17353104	3
Caelo	Magnesium hydrogen citrate	17353104P-180831-2	1
Caelo	Magnesium hydrogen citrate	17353104P-181001-2	1
Caelo	Magnesium hydrogen citrate	17353105	1
Caelo	Magnesium hydrogen citrate	17353109	1
Caelo	Magnesium hydrogen citrate	1811038-01	2
Caelo	Magnesium hydrogen citrate	18216803	4
Caelo	Magnesium hydrogen citrate	18216803P-181218-1	1
Caelo	Magnesium hydrogen citrate	18216803P-190225-5	1
Caelo	Magnesium hydrogen citrate	18216804	3
Caelo	Magnesium hydrogen citrate	18216804P-190325-1	1
Caelo	Magnesium hydrogen citrate	18216804P-191004-1	1
Caelo	Magnesium hydrogen citrate	18216806	6
Caelo	Magnesium hydrogen citrate	18274601	1
Caelo	Magnesium hydrogen citrate	18274602	1
Caelo	Magnesium hydrogen citrate	18274603	2
Caelo	Magnesium hydrogen citrate	18274604	3
Caelo	Magnesium hydrogen citrate	18274606	3
Caelo	Magnesium hydrogen citrate	18274606P-200331-3	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Magnesium hydrogen citrate	18274609	2
Caelo	Magnesium hydrogen citrate	18274610	1
Caelo	Magnesium hydrogen citrate	18274612	1
Caelo	Magnesium hydrogen citrate	18A08-B04-345115	1
Caelo	Magnesium hydrogen citrate	19000684001	2
Caelo	Magnesium hydrogen citrate	19000684002	4
Caelo	Magnesium hydrogen citrate	19000684003	3
Caelo	Magnesium hydrogen citrate	1904011-01	3
Caelo	Magnesium hydrogen citrate	19061316	1
Caelo	Magnesium hydrogen citrate	20002495002	2
Caelo	Magnesium hydrogen citrate	20002495003	4
Caelo	Magnesium hydrogen citrate	20002495006	2
Caelo	Magnesium hydrogen citrate	20002495010	1
Caelo	Magnesium hydrogen citrate	21000135002	1
Caelo	Magnesium hydrogen citrate	21000135005	1
Caelo	Magnesium hydrogen citrate	21000135006	1
Caelo	Magnesium hydrogen citrate	21000135007	2
Caelo	Magnesium hydrogen citrate	21000135011	1
Caelo	Magnesium hydrogen citrate	21003604004	7
Caelo	Magnesium hydrogen citrate	218U-01829	1
Caelo	Magnesium hydrogen citrate	2368011	1
Caelo	Magnesium hydrogen citrate	26101203	1
Caelo	Magnesium hydrogen citrate	27101704	1
Caelo	Magnesium hydrogen citrate	27111306	1
Caelo	Magnesium hydrogen citrate	315E-01829	1
Caelo	Magnesium hydrogen citrate	411052-2-P	1
Caelo	Magnesium hydrogen citrate	516Q-01829	1
Caelo	Magnesium hydrogen citrate	6081301	1
Caelo	Magnesium hydrogen citrate	7011504	1
Caelo	Magnesium hydrogen citrate	80446188	1
Caelo	Magnesium hydrogen citrate	90396169	1
Caelo	Magnesium hydrogen citrate	913M-01829	1
Caeol/Noweda	Magnesium hydrogen citrate	17353105	1
Caeolo/Gehe	Magnesium hydrogen citrate	17173405	2
Caesar & Loretz GmbH...	Magnesium hydrogen citrate	18274602	1
Caesar & Loretz GmbH...	Magnesium hydrogen citrate	18274601	1
Caesar & Loretz GmbH...	Magnesium hydrogen citrate	18274609	1
Caesar & Loretz GmbH...	Magnesium hydrogen citrate	19000684004	1
Caesar & Loretz GmbH...	Magnesium hydrogen citrate	19000684002	1
Caesar & Loretz GmbH...	Magnesium hydrogen citrate	20002495003	1
Caesar & Loretz GmbH...	Magnesium hydrogen citrate	18274609	1
Caesar & Loretz GmbH/Ph	Magnesium hydrogen citrate	20002495003	1
Caesar & Loretz GmbH...	Magnesium hydrogen citrate	20002495002	1
Caesar & Loretz GmbH...	Magnesium hydrogen citrate	21000135006	1
Caesar & Loretz GmbH	Magnesium hydrogen citrate	17353109	1
Caesar & Loretz GmbH	Magnesium hydrogen citrate	18216803	1
Caesar & Loretz GmbH	Magnesium hydrogen citrate	18274602	1
Caesar & Loretz GmbH	Magnesium hydrogen citrate	18274604	3
Caesar & Loretz GmbH	Magnesium hydrogen citrate	18274605	1
Caesar & Loretz GmbH	Magnesium hydrogen citrate	18274609	1
Caesar & Loretz GmbH	Magnesium hydrogen citrate	18274610	3
Caesar & Loretz GmbH	Magnesium hydrogen citrate	19000684003	1
Caesar & Loretz GmbH	Magnesium hydrogen citrate	20002495001	2
Caesar & Loretz GmbH	Magnesium hydrogen citrate	20002495002	2
Caesar & Loretz GmbH	Magnesium hydrogen citrate	20002495003	2
Caesar & Loretz	Magnesium hydrogen citrate	16341711	1
Caleo/ Noweda	Magnesium hydrogen citrate	18216803	1
Cealo	Magnesium hydrogen citrate	12368014	1
Cealo	Magnesium hydrogen citrate	13233907	2
Dr. Paul Lohmann	Magnesium hydrogen citrate	1077866	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Dr. Paul Lohmann	Magnesium hydrogen citrate	1078434	1
Dr. Paul Lohmann	Magnesium hydrogen citrate	1079474	1
Eu Rho	Magnesium hydrogen citrate	110600401	1
Eu Rho	Magnesium hydrogen citrate	1202034-01	1
Eu Rho	Magnesium hydrogen citrate	1306034-01	1
EuRho/Phönix	Magnesium hydrogen citrate	1202034-02	1
EuRho/Phönix	Magnesium hydrogen citrate	1311003-01	1
EuRho	Magnesium hydrogen citrate	1311003-02	1
EuRho	Magnesium hydrogen citrate	1507010-02	1
EuRho	Magnesium hydrogen citrate	1910005-01	1
Euro OTC	Magnesium hydrogen citrate		3
Euro OTC	Magnesium hydrogen citrate	1080144	1
Euro OTC	Magnesium hydrogen citrate	1085730	2
Euro OTC	Magnesium hydrogen citrate	1110026-01	2
Euro OTC	Magnesium hydrogen citrate	1208006-01	3
Euro OTC	Magnesium hydrogen citrate	120800602	1
Euro OTC	Magnesium hydrogen citrate	1211033-01	4
Euro OTC	Magnesium hydrogen citrate	1211033-02	4
Euro OTC	Magnesium hydrogen citrate	1306034-01	2
Euro OTC	Magnesium hydrogen citrate	130603402	1
Euro OTC	Magnesium hydrogen citrate	1306034-02	2
Euro OTC	Magnesium hydrogen citrate	1311003-01	7
Euro OTC	Magnesium hydrogen citrate	1311003-02	1
Euro OTC	Magnesium hydrogen citrate	140402301	1
Euro OTC	Magnesium hydrogen citrate	1404023-01	5
Euro OTC	Magnesium hydrogen citrate	140704801	1
Euro OTC	Magnesium hydrogen citrate	1407048-01	4
Euro OTC	Magnesium hydrogen citrate	1407048-02	3
Euro OTC	Magnesium hydrogen citrate	1501026-01	5
Euro OTC	Magnesium hydrogen citrate	1507010-01	10
Euro OTC	Magnesium hydrogen citrate	1507010-02	2
Euro OTC	Magnesium hydrogen citrate	151003301	2
Euro OTC	Magnesium hydrogen citrate	1510033-01	2
Euro OTC	Magnesium hydrogen citrate	16000456/0	1
Euro OTC	Magnesium hydrogen citrate	160100501	1
Euro OTC	Magnesium hydrogen citrate	1601005-01	18
Euro OTC	Magnesium hydrogen citrate	1604002-001	1
Euro OTC	Magnesium hydrogen citrate	1604002-01	34
Euro OTC	Magnesium hydrogen citrate	1604002-012x	1
Euro OTC	Magnesium hydrogen citrate	1604002-02	8
Euro OTC	Magnesium hydrogen citrate	160800401	2
Euro OTC	Magnesium hydrogen citrate	1608004-01	22
Euro OTC	Magnesium hydrogen citrate	1608004-02	2
Euro OTC	Magnesium hydrogen citrate	1701003-01	7
Euro OTC	Magnesium hydrogen citrate	170100401	1
Euro OTC	Magnesium hydrogen citrate	1701004-01	4
Euro OTC	Magnesium hydrogen citrate	17050009-01	1
Euro OTC	Magnesium hydrogen citrate	1705009-01	5
Euro OTC	Magnesium hydrogen citrate	1705010-01	7
Euro OTC	Magnesium hydrogen citrate	1710001-01	1
Euro OTC	Magnesium hydrogen citrate	171000701	1
Euro OTC	Magnesium hydrogen citrate	1710007-01	10
Euro OTC	Magnesium hydrogen citrate	1710007-02	1
Euro OTC	Magnesium hydrogen citrate	17353105	1
Euro OTC	Magnesium hydrogen citrate	1802026-01	6
Euro OTC	Magnesium hydrogen citrate	1808006-01	5
Euro OTC	Magnesium hydrogen citrate	1811038-01	11
Euro OTC	Magnesium hydrogen citrate	190401101	2
Euro OTC	Magnesium hydrogen citrate	1904011-01	15
Euro OTC	Magnesium hydrogen citrate	190702001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Magnesium hydrogen citrate	1907020-01	7
Euro OTC	Magnesium hydrogen citrate	1910005-01	7
Euro OTC	Magnesium hydrogen citrate	2003064-01	8
Euro OTC	Magnesium hydrogen citrate	2005027-01	14
Euro OTC	Magnesium hydrogen citrate	2009007-01	15
Euro OTC	Magnesium hydrogen citrate	2101004-01	2
Euro OTC	Magnesium hydrogen citrate	2104021-01	1
Euro OTC	Magnesium hydrogen citrate	2110009-01	3
Euro OTC	Magnesium hydrogen citrate	2114M1829	1
Euro OTC	Magnesium hydrogen citrate	220100401	1
Euro OTC	Magnesium hydrogen citrate	2201004-01	6
Euro OTC	Magnesium hydrogen citrate	2206017-01	6
Euro OTC	Magnesium hydrogen citrate	3030559	1
Euro OTC	Magnesium hydrogen citrate	3035708	1
Euro OTC	Magnesium hydrogen citrate	3068048	1
Fagron	Magnesium hydrogen citrate		1
Fagron	Magnesium hydrogen citrate	1056239	1
Fagron	Magnesium hydrogen citrate	1087537	1
Fagron	Magnesium hydrogen citrate	11H05-N07	1
Fagron	Magnesium hydrogen citrate	12G10-N01	2
Fagron	Magnesium hydrogen citrate	13B22-N03	1
Fagron	Magnesium hydrogen citrate	13D30-N07	2
Fagron	Magnesium hydrogen citrate	13K11-B02-288161	1
Fagron	Magnesium hydrogen citrate	13K11-BO2-288161	1
Fagron	Magnesium hydrogen citrate	14/12-B02-298854	1
Fagron	Magnesium hydrogen citrate	14I12-B02	1
Fagron	Magnesium hydrogen citrate	14I12-B02-298854	1
Fagron	Magnesium hydrogen citrate	14K-B03-305254	1
Fagron	Magnesium hydrogen citrate	15296701	1
Fagron	Magnesium hydrogen citrate	16E02-B03-0326874	1
Fagron	Magnesium hydrogen citrate	16E02-B03-326874	1
Fagron	Magnesium hydrogen citrate	17G24-B03-338029	2
Fagron	Magnesium hydrogen citrate	17G24-B03-341019	1
Fagron	Magnesium hydrogen citrate	18/20-B06	1
Fagron	Magnesium hydrogen citrate	18A08-B04-345115	1
Fagron	Magnesium hydrogen citrate	18A08-B04-345155	1
Fagron	Magnesium hydrogen citrate	18A08-B04-349372	1
Fagron	Magnesium hydrogen citrate	18I20-B06-355658	1
Fagron	Magnesium hydrogen citrate	20A17-B08-196635	2
Fagron	Magnesium hydrogen citrate	20A17-B08-200819	1
Fagron	Magnesium hydrogen citrate	20I25-B03-201926	1
Fagron	Magnesium hydrogen citrate	3047166	2
Fagron	Magnesium hydrogen citrate	B07-2136601	1
Fiebig	Magnesium hydrogen citrate	1802026-01	1
Gatt-Koller	Magnesium hydrogen citrate		1
Gatt-Koller	Magnesium hydrogen citrate	1800208	1
Gatt-Koller	Magnesium hydrogen citrate	1802721	1
Gatt-Koller	Magnesium hydrogen citrate	1803714	2
Gehe Kassel	Magnesium hydrogen citrate	14/12-B02-298854	1
GEHE	Magnesium hydrogen citrate	1802026-01	1
Heidelberger Chlorel…	Magnesium hydrogen citrate	10032	1
Heidelberger Chlorella	Magnesium hydrogen citrate	90196	1
Ichthyol/Phönix	Magnesium hydrogen citrate	14/12-B02-298854	1
INTERN-DROGEN	Magnesium hydrogen citrate	210001350007	1
INTERN-DROGEN	Magnesium hydrogen citrate	21000135006	1
Kehr	Magnesium hydrogen citrate	17173406	1
kögl	Magnesium hydrogen citrate	1900910	1
L30	Magnesium hydrogen citrate	1608004-01	1
lohmann	Magnesium hydrogen citrate	3054132	1
Nachprüfung vom 31.1…	Magnesium hydrogen citrate	16341710	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Nowed18.08.2015	Magnesium hydrogen citrate	14265521	1
Noweda	Magnesium hydrogen citrate	10163306	1
Noweda	Magnesium hydrogen citrate	16341710	1
Noweda	Magnesium hydrogen citrate	18274603	1
Noweda	Magnesium hydrogen citrate	2005027-01	1
Noweda	Magnesium hydrogen citrate	22002876002	1
Noweda	Magnesium hydrogen citrate	2206017-01	1
Phoenix 15.10.14	Magnesium hydrogen citrate	1311003-01	1
Phönix	Magnesium hydrogen citrate	1211033-01	2
phönix	Magnesium hydrogen citrate	15296702	1
phönix	Magnesium hydrogen citrate	15296710	1
Phönix	Magnesium hydrogen citrate	15415005	1
phönix	Magnesium hydrogen citrate	15415010	1
phönix	Magnesium hydrogen citrate	15415015	2
phönix	Magnesium hydrogen citrate	1601005-01	2
phönix	Magnesium hydrogen citrate	1604002-01	1
phönix	Magnesium hydrogen citrate	1608004-01	1
phönix	Magnesium hydrogen citrate	16341709	2
Sanacaorp	Magnesium hydrogen citrate	13389108	1
Sanacorp	Magnesium hydrogen citrate	16341710	1
Sanacorp	Magnesium hydrogen citrate	20002495003	1
Sanacorp	Magnesium hydrogen citrate	20A17-B08-196635	1
Sanacorp	Magnesium hydrogen citrate	22001882001	1
Sanacorp	Magnesium hydrogen citrate	2304016-01	1
Sanacorp	Magnesium hydrogen citrate	3108363	1
VDL;27.02.15	Magnesium hydrogen citrate	13389111	1

- 235 256 spectra from 1515 *Apo-Ident* customers from a total of 49 007 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Magnesium hydrogen citrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Magnesium hydrogen citrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	540	0	152 422
Type B	0	1490	0	200 594
Type C	0	810	1	235 256

The substance/substance group *Magnesium hydrogen citrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8889 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.5973 %)
Type C	100.0000 % (> 99.9007 %)	99.8767 % (> 99.5068 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21445	22233	5.57	88.08
21873	21873	0.00	86.27
22233	22233	0.00	87.51
22296	22296	0.00	87.45
22992	22992	0.00	85.89
23240	22992	4.21	85.88
25545	25545	0.00	94.75
26251	26251	0.00	78.03
26400	26400	0.00	114.13
26423	26423	0.00	90.20
27302	21873	40.54	99.56

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Magnesium orotate dihydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20429-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Magnesium orotate dihydrate; Magnesii orotas dihydricus

Special notes

When selecting the *Magnesium orotate dihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Magnesium orotate dihydrate	7	17	36

Second-stage model

For differentiation of the substance/substance group *Magnesium orotate dihydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Magnesium orotate dihydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Manganese orotate dihydrate	76.61	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Magnesium orotate dihydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Magnesium orotate dihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Magnesium orotate dihydrate	162227	22638	40	20160809*
Caelo	Magnesium orotate dihydrate	16222701	23236	40	20160809
Euro OTC	Magnesium orotate dihydrate	1511021	22287	60	20151228*
Euro OTC	Magnesium orotate dihydrate	1707018	23615	40	20170907*
Euro OTC	Magnesium orotate dihydrate	1911024	25069	40	20200107*
Euro OTC	Magnesium orotate dihydrate	2003014	25147	40	20200416*
Euro OTC	Magnesium orotate dihydrate	2309021	26926	40	20231011*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 300 spectra of 7 reference samples from the substance/substance group *Magnesium orotate dihydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 662 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 750 spectra of 21 reference samples from the substance/substance group *Magnesium orotate dihydrate*.

- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Magnesium orotate dihydrate	172157	23661	40
Caelo	Magnesium orotate dihydrate	172547	23799	40
Euro OTC	Magnesium orotate dihydrate	1608017	22784	40
Euro OTC	Magnesium orotate dihydrate	1712001	23874	40
Euro OTC	Magnesium orotate dihydrate	1802018	23963	40
Euro OTC	Magnesium orotate dihydrate	1808029	24200	40
Euro OTC	Magnesium orotate dihydrate	1902007	24490	40
Euro OTC	Magnesium orotate dihydrate	1906014	24797	40
Euro OTC	Magnesium orotate dihydrate	1909007	24835	40
Euro OTC	Magnesium orotate dihydrate	2006004	25341	40
Euro OTC	Magnesium orotate dihydrate	2102003	25595	40
Euro OTC	Magnesium orotate dihydrate	2109023	25892	50
Euro OTC	Magnesium orotate dihydrate	2202010	25969	40
Euro OTC	Magnesium orotate dihydrate	2207009	26196	40
Euro OTC	Magnesium orotate dihydrate	2301041	26584	40
Euro OTC	Magnesium orotate dihydrate	2403014	27214	40
Euro OTC	Magnesium orotate dihydrate	2408014	27399	40
Euro OTC	Magnesium orotate dihydrate	2109023	25892SI	10
Euro OTC	Magnesium orotate dihydrate	2202010	25969SI	10
Euro OTC	Magnesium orotate dihydrate	2207009	26196SI	20
Euro OTC	Magnesium orotate dihydrate	2301041	26584SI	20

- 201 334 spectra from a total of 4028 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 62 spectra from 25 *Apo-Ident* customers from 36 batches from the substance/substance group *Magnesium orotate dihydrate*.
- Among them are spectra of independent samples from 36 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Magnesium orotate dihydrate	14093607	2
Caelo	Magnesium orotate dihydrate	1808029-01	1
EuRho	Magnesium orotate dihydrate	2102003-01	1
Euro OTC	Magnesium orotate dihydrate	1209029-01	3
Euro OTC	Magnesium orotate dihydrate	1305011-01	1
Euro OTC	Magnesium orotate dihydrate	130501102	1
Euro OTC	Magnesium orotate dihydrate	1305011-02	5
Euro OTC	Magnesium orotate dihydrate	1407005-01	3
Euro OTC	Magnesium orotate dihydrate	1504002-01	1
Euro OTC	Magnesium orotate dihydrate	1504002-02	1
Euro OTC	Magnesium orotate dihydrate	151102101	1
Euro OTC	Magnesium orotate dihydrate	1511021-02	6
Euro OTC	Magnesium orotate dihydrate	1608017-01	2
Euro OTC	Magnesium orotate dihydrate	1608017-02	1
Euro OTC	Magnesium orotate dihydrate	16085017-01	1
Euro OTC	Magnesium orotate dihydrate	1707018-01	4
Euro OTC	Magnesium orotate dihydrate	1712001-01	2
Euro OTC	Magnesium orotate dihydrate	1802018-01	1
Euro OTC	Magnesium orotate dihydrate	1808029-01	1
Euro OTC	Magnesium orotate dihydrate	180802902	1
Euro OTC	Magnesium orotate dihydrate	1906014-01	2
Euro OTC	Magnesium orotate dihydrate	1909007-01	2
Euro OTC	Magnesium orotate dihydrate	2003014-01	2
Euro OTC	Magnesium orotate dihydrate	2006004-01	1
Euro OTC	Magnesium orotate dihydrate	2102003-01	1
Euro OTC	Magnesium orotate dihydrate	2109023-01	1
Euro OTC	Magnesium orotate dihydrate	2109023-02	1
Fagron	Magnesium orotate dihydrate	1000060461	1
Fagron	Magnesium orotate dihydrate	12G05-N03	1
Fagron	Magnesium orotate dihydrate	13H06-N07	1
Fagron	Magnesium orotate dihydrate	14/13-B05-305616	1
Fagron	Magnesium orotate dihydrate	14E20-B05-296005	1
Fagron	Magnesium orotate dihydrate	160801701	1
Fagron	Magnesium orotate dihydrate	16K22B01329783	1
Fagron	Magnesium orotate dihydrate	17H14-B02	1
Fagron	Magnesium orotate dihydrate	17H14B02346538	1
Fagron	Magnesium orotate dihydrate	354317	1
Noweda	Magnesium orotate dihydrate	2109023-01	2
Noweda	Magnesium orotate dihydrate	2301041-01	1

- 236 005 spectra from 1515 *Apo-Ident* customers from a total of 49 223 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Magnesium orotate dihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Magnesium orotate dihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	750	0	201 334
Type C	0	62	0	236 005

The substance/substance group *Magnesium orotate dihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 90.3226 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22287	22287	0.00	139.36
22638	22638	0.00	153.66
23236	22638	7.68	154.31
23615	23615	0.00	142.22
25069	25069	0.00	151.51
25147	25147	0.00	150.78
26926	26926	0.00	143.47

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Magnesium stearate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20707-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Magnesium stearate; Magnesii stearas

Special notes

When selecting the *Magnesium stearate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Magnesium stearate	7	10	34

Second-stage model

For differentiation of the substance/substance group *Magnesium stearate* the following second-stage model is used:

- Submodel 01

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Magnesium stearate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cetyl palmitate	51.79	15.37
⋮	⋮	⋮
Beeswax, white	>50	19.46
Hard fat W35	>50	20.81
Hard fat	>50	22.16
Paraffin, hard	>50	25.83
Beeswax, yellow	>50	29.49
Cocoa butter	>50	32.14
Paraffin, microcrystalline	>50	36.27
Sodium dodecyl sulfate	>50	40.52

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Magnesium stearate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Magnesium stearate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Magnesium stearate	13095536	21117	40	20130405
Caelo	Magnesium stearate	14136929	21783	60	AR-15-FG-012028-01
Euro OTC	Magnesium stearate	1502033-01	22817	40	20150317
Euro OTC	Magnesium stearate	1704002	23436	40	20170622*
Euro OTC	Magnesium stearate	2301035	26649	40	20230323*
Euro OTC	Magnesium stearate	2301035	26649SI	20	20230323*
Fagron	Magnesium stearate	12C29-N06	20707	110	20120418
Fagron	Magnesium stearate	12D26-B03	21084	40	1407310

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 390 spectra of 8 reference samples from the substance/substance group *Magnesium stearate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 572 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 440 spectra of 12 reference samples from the substance/substance group *Magnesium stearate*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Magnesium stearate	162066	22763	40
Caelo	Magnesium stearate	181533	24215	40
Caelo	Magnesium stearate	183089	24354	40
Caelo	Magnesium stearate	192527	24897	40
Caelo	Magnesium stearate	21004078013	26743	40
Caelo	Magnesium stearate	23002099	26973	40
Euro OTC	Magnesium stearate	1608022	22821	40
Euro OTC	Magnesium stearate	1901033	24459	40
Euro OTC	Magnesium stearate	2009032	25398	40
Euro OTC	Magnesium stearate	2109010	25886	50
Caelo	Magnesium stearate	21004078013	26743SI	20
Euro OTC	Magnesium stearate	2109010	25886SI	10

- 201 644 spectra from a total of 4035 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 65 spectra from 48 *Apo-Ident* customers from 36 batches from the substance/substance group *Magnesium stearate*.
- Among them are spectra of independent samples from 34 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Magnesium stearate	21004078005	1
	Magnesium stearate	2100407813	1
	Magnesium stearate	23000572003	2
Caelo	Magnesium stearate	12040307	1
Caelo	Magnesium stearate	13095515	1
Caelo	Magnesium stearate	13095536	1
Caelo	Magnesium stearate	15155001	2
Caelo	Magnesium stearate	15305302	3
Caelo	Magnesium stearate	15305307	1
Caelo	Magnesium stearate	15305315	4
Caelo	Magnesium stearate	15305323	1
Caelo	Magnesium stearate	16206602	3
Caelo	Magnesium stearate	16206610	7
Caelo	Magnesium stearate	16206617	1
Caelo	Magnesium stearate	17360006	2
Caelo	Magnesium stearate	18153310	2
Caelo	Magnesium stearate	183038912	1
Caelo	Magnesium stearate	18308912	1
Caelo	Magnesium stearate	18308916	2
Caelo	Magnesium stearate	192527003	1
Caelo	Magnesium stearate	192527006	1
Caelo	Magnesium stearate	20004065001	2
Caesar & Loretz GmbH...	Magnesium stearate	15322002	1
Caesar & Loretz GmbH/Kehr	Magnesium stearate	18153310	1
Caesar & Loretz GmbH...	Magnesium stearate	18153310	1
Caesar & Loretz GmbH	Magnesium stearate	18308912	1
Caesar & Loretz GmbH	Magnesium stearate	18308916	1
Caesar & Loretz GmbH	Magnesium stearate	192527003	1
Caesar & Loretz GmbH	Magnesium stearate	20004065001	1
Euro OTC	Magnesium stearate	1116E-01834	1
Euro OTC	Magnesium stearate	1119I-01834	1
Euro OTC	Magnesium stearate	1502033-01	2
Euro OTC	Magnesium stearate	1912I-01834	1
Euro OTC	Magnesium stearate	2009032-01	1
Euro OTC	Magnesium stearate	315E-01834	1
Euro OTC	Magnesium stearate	718I-01834	1
Euro OTC	Magnesium stearate	914I-01834	1
Fagron	Magnesium stearate	12D26-B03-289435	1
FL Apotheke	Magnesium stearate	xxxxxx	1
Jenne	Magnesium stearate	21004078010	1
Noweda	Magnesium stearate	21004078013	1
Phoenix	Magnesium stearate	23000572003	1
ROHA	Magnesium stearate	130230	1
Sanacorp	Magnesium stearate	21004078013	1
Sanacorp	Magnesium stearate	23000572003	1

- 236 002 spectra from 1515 *Apo-Ident* customers from a total of 49 223 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Magnesium stearate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Magnesium stearate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	390	0	152 572
Type B	0	440	0	201 644
Type C	0	65	0	236 002

The substance/substance group *Magnesium stearate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4615 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6364 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 90.7692 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20707	21783	54.93	106.34
21084	21084	0.00	134.05
21117	26649	26.21	129.88
21783	21783	0.00	139.76
22817	21783	5.71	139.16
23436	23436	0.00	133.97
26649	26649	0.00	132.63

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Magnesium sulfate heptahydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20165-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Magnesium sulfate heptahydrate; Magnesii sulfas heptahydricus; Magnesium sulphate heptahydrate

Special notes

When selecting the *Magnesium sulfate heptahydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Magnesium sulfate heptahydrate	6	2	52

Second-stage model

For differentiation of the substance/substance group *Magnesium sulfate heptahydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Magnesium sulfate heptahydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Zinc sulfate heptahydrate	34.24	–
Sodium cromoglicate	50.93	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Magnesium sulfate heptahydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Magnesium sulfate heptahydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Magnesium sulfate heptahydrate	22000334	26054	40	20220301*
Caelo	Magnesium sulfate heptahydrate	21002002	26055	40	20210923*
Caelo	Magnesium sulfate heptahydrate	22003020	26561	40	20221207*
Caelo	Magnesium sulfate heptahydrate	22003020	26561SI	20	20221207*
Caelo	Magnesium sulfate heptahydrate	23003364	27105	40	20240124*
Caelo	Magnesium sulfate heptahydrate	24002186	27431	40	20241011*
Euro OTC	Magnesium sulfate heptahydrate	2308013	26882	40	20230829*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 260 spectra of 7 reference samples from the substance/substance group *Magnesium sulfate heptahydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 110 spectra of 4 reference samples from the substance/substance group *Magnesium sulfate heptahydrate*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Magnesium sulfate heptahydrate	23001612	26849	40
Euro OTC	Magnesium sulfate heptahydrate	2107026	25789	50
Caelo	Magnesium sulfate heptahydrate	22000334	26054SI†	10
Caelo	Magnesium sulfate heptahydrate	21002002	26055SI†	10

- 201 974 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 126 spectra from 65 *Apo-Ident* customers from 52 batches from the substance/substance group *Magnesium sulfate heptahydrate*.

- Among them are spectra of independent samples from 52 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Magnesium sulfate heptahydrate	1401029-01	1
	Magnesium sulfate heptahydrate	21002002005	1
	Magnesium sulfate heptahydrate	22001077002	4
	Magnesium sulfate heptahydrate	22003025001	2
	Magnesium sulfate heptahydrate	22003025003	10
	Magnesium sulfate heptahydrate	2210012-01	2
	Magnesium sulfate heptahydrate	3134859	1
Anzag 29.04.13 ek: 4,55EUR	Magnesium sulfate heptahydrate	12138518	1
Anzag	Magnesium sulfate heptahydrate	204035	1
BfB	Magnesium sulfate heptahydrate	12L10-N07	2
Bombastus	Magnesium sulfate heptahydrate	277424	1
Caelo	Magnesium sulfate heptahydrate	10104201	1
Caelo	Magnesium sulfate heptahydrate	10371111	1
Caelo	Magnesium sulfate heptahydrate	11194001	1
Caelo	Magnesium sulfate heptahydrate	11369252	1
Caelo	Magnesium sulfate heptahydrate	11369509	1
Caelo	Magnesium sulfate heptahydrate	11369525	6
Caelo	Magnesium sulfate heptahydrate	11369526	12
Caelo	Magnesium sulfate heptahydrate	11369529	1
Caelo	Magnesium sulfate heptahydrate	113695625	1
Caelo	Magnesium sulfate heptahydrate	1206019-01	4
Caelo	Magnesium sulfate heptahydrate	12119901/2	1
Caelo	Magnesium sulfate heptahydrate	12138518	2
Caelo	Magnesium sulfate heptahydrate	12138521	2
Caelo	Magnesium sulfate heptahydrate	1213E-01835	1
Caelo	Magnesium sulfate heptahydrate	12336914	5
Caelo	Magnesium sulfate heptahydrate	12336915	3
Caelo	Magnesium sulfate heptahydrate	12336926	1
Caelo	Magnesium sulfate heptahydrate	12c27-n06	1
Caelo	Magnesium sulfate heptahydrate	13030104	1
Caelo	Magnesium sulfate heptahydrate	13030107	1
Caelo	Magnesium sulfate heptahydrate	13183702	2
Caelo	Magnesium sulfate heptahydrate	6012014B	1
Caelo	Magnesium sulfate heptahydrate	90744129	1
EuRho/Jenne	Magnesium sulfate heptahydrate	1202017-01	1
EuRho	Magnesium sulfate heptahydrate	1206019-01	1
EuRho	Magnesium sulfate heptahydrate	1303008-01	2
EuRho	Magnesium sulfate heptahydrate	3512M-01835	1
Euro / Jenne	Magnesium sulfate heptahydrate	1401029-01	1
Euro OTC	Magnesium sulfate heptahydrate	1109023-01	1
Euro OTC	Magnesium sulfate heptahydrate	1202017-01	5
Euro OTC	Magnesium sulfate heptahydrate	1211022-01	3
Euro OTC	Magnesium sulfate heptahydrate	130300801	1
Euro OTC	Magnesium sulfate heptahydrate	1303008-01	3
Euro OTC	Magnesium sulfate heptahydrate	1306015-01	1
Euro OTC	Magnesium sulfate heptahydrate	170610	1
Fagron	Magnesium sulfate heptahydrate	12E22-N02	3
Fagron	Magnesium sulfate heptahydrate	12G24-N02	1
Fagron	Magnesium sulfate heptahydrate	12L10-N07	6
Fagron	Magnesium sulfate heptahydrate	12L10-NO7	1
Fagron	Magnesium sulfate heptahydrate	13H05-N02	1
Fagron	Magnesium sulfate heptahydrate	26251	1
Fagron	Magnesium sulfate heptahydrate	31161	1
fargon	Magnesium sulfate heptahydrate	12E22-N02	1
Gehe	Magnesium sulfate heptahydrate	12138521	2
Gehe	Magnesium sulfate heptahydrate	21002002001	1
Hedinger	Magnesium sulfate heptahydrate	204036	1
Hedinger	Magnesium sulfate heptahydrate	204037	2
Noweda / 28.10.13 EuRho	Magnesium sulfate heptahydrate	1211022-01	1
Noweda	Magnesium sulfate heptahydrate	1109023-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Magnesium sulfate heptahydrate	22003025001	1
Phoenix	Magnesium sulfate heptahydrate	24000129002	1
Phönix	Magnesium sulfate heptahydrate	11369526	1
Phönix	Magnesium sulfate heptahydrate	22000333004	1
Sanacorp	Magnesium sulfate heptahydrate	22003025001	1

- 235 941 spectra from 1515 *Apo-Ident* customers from a total of 49 207 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Magnesium sulfate heptahydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Magnesium sulfate heptahydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	110	0	201 974
Type C	0	126	0	235 941

The substance/substance group *Magnesium sulfate heptahydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 94.5455 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 95.2381 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26054	26054	0.00	68.75
26055	26055	0.00	140.36
26561	26561	0.00	66.05
26882	26882	0.00	74.40
27105	27105	0.00	87.07
27431	27431	0.00	77.02

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Maltodextrin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20709-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Maltodextrin; Maltodextrinum

Special notes

When selecting the *Maltodextrin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Maltodextrin	2	1	3

Second-stage model

For differentiation of the substance/substance group *Maltodextrin* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Maltodextrin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Rice starch	23.97	15.60
SyrSpend® SF pH4 neo (Maize starch)	26.64	13.17
SyrSpend® SF pH4	32.86	20.56
Wheat starch	33.68	17.24
Corn starch	35.80	24.18
SyrSpend® SF Alka	41.62	18.57
Acacia, dried dispersion	54.36	30.27
⋮	⋮	⋮
Potato starch	>50	19.16
Carmellose sodium	>50	25.12
Colistin sulfate	>50	30.09
Polymyxin B sulfate	>50	36.46
Calcium glycerophosphate	>50	44.23
Amphotericin B	>50	49.98
Bacitracin	>50	56.46
Riboflavin	>50	62.26
Cyanocobalamin	>50	67.39
Tosylchloramide sodium	>50	77.62
Selenium yeast	>50	78.34
Fructose	>50	83.56
Calcium pantothenate	>50	86.25
Nystatin	>50	90.48
Oxalic acid	>50	105.58
Gelatine, white	>50	108.39
Hyoscine hydrobromide	>50	118.56
Estradiol hemihydrate	>50	125.62
Triamcinolone	>50	136.33
alpha-tocopheryl acetate dry concentrate	>50	142.86
Estriol	>50	175.56
Methylcobalamin	>50	186.75

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Maltodextrin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Maltodextrin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Gatt-Koller	Maltodextrin	21J01645	26382	40	20210909
Gatt-Koller	Maltodextrin	21J01645	26382SI	20	20210909
Inresa	Maltodextrin	R1503902	21806	60	AR-15-FG-008821-01

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 120 spectra of 3 reference samples from the substance/substance group *Maltodextrin*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

- 152 842 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 60 spectra of 1 reference samples from the substance/substance group *Maltodextrin*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Inresa	Maltodextrin	R1600014	22314	60

- 202 024 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5 spectra from 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Maltodextrin*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
HBK Gesundheit	Maltodextrin	1143	3
HBK Gesundheit	Maltodextrin	2343	1
Phönix	Maltodextrin	LOT20250206JB	1

- 236 062 spectra from 1515 *Apo-Ident* customers from a total of 49 255 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Maltodextrin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Maltodextrin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	120	0	152 842
Type B	0	60	0	202 024
Type C	0	5	0	236 062

The substance/substance group *Maltodextrin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21806	21806	0.00	42.05
26382	21806	14.43	43.54

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Manganese orotate dihydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	22311-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Manganese orotate dihydrate

Special notes

When selecting the *Manganese orotate dihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Manganese orotate dihydrate	5	2	1

Second-stage model

For differentiation of the substance/substance group *Manganese orotate dihydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Manganese orotate dihydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Magnesium orotate dihydrate	83.14	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Manganese orotate dihydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Manganese orotate dihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Manganese orotate dihydrate	1601003	22311	60	20160113*
Euro OTC	Manganese orotate dihydrate	1801031	23908	40	20180131*
Euro OTC	Manganese orotate dihydrate	1907009	24787	40	20190718*
Euro OTC	Manganese orotate dihydrate	2208027	26265	40	20220905*
Euro OTC	Manganese orotate dihydrate	2311027	27073	40	20231221*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 220 spectra of 5 reference samples from the substance/substance group *Manganese orotate dihydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 742 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 5 reference samples from the substance/substance group *Manganese orotate dihydrate*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Manganese orotate dihydrate	1605029-01	22654	40
Euro OTC	Manganese orotate dihydrate	2010007	25466	40
Euro OTC	Manganese orotate dihydrate	1605029-01	22737	40
Euro OTC	Manganese orotate dihydrate	2208027	26265SI†	20
Euro OTC	Manganese orotate dihydrate	2311027	27073SI†	20

- 201 924 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Manganese orotate dihydrate*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Manganese orotate dihydrate	1907009-02	1

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Manganese orotate dihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Manganese orotate dihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	220	0	152 742
Type B	0	160	0	201 924
Type C	0	1	0	236 066

The substance/substance group *Manganese orotate dihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22311	22311	0.00	163.70
23908	23908	0.00	146.77
24787	24787	0.00	145.40
26265	26265	0.00	162.33
27073	27073	0.00	165.96

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Manganese sulfate monohydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20404-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Manganese sulfate monohydrate; Manganese sulphate monohydrate; Mangani sulfas monohydricus

Special notes

When selecting the *Manganese sulfate monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Manganese sulfate monohydrate	2	1	0

Second-stage model

For differentiation of the substance/substance group *Manganese sulfate monohydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Manganese sulfate monohydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	81.92	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Manganese sulfate monohydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Manganese sulfate monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Manganese sulfate monohydrate	171648	24404	40	20170714*
Euro OTC	Manganese sulfate monohydrate	2305003	26771	40	20230630*
Euro OTC	Manganese sulfate monohydrate	2305003	26771SI	20	20230630*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 100 spectra of 3 reference samples from the substance/substance group *Manganese sulfate monohydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 862 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 50 spectra of 2 reference samples from the substance/substance group *Manganese sulfate monohydrate*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Manganese sulfate monohydrate	2202003	26047	40
Euro OTC	Manganese sulfate monohydrate	2202003	26047SI	10

- 202 034 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Manganese sulfate monohydrate*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Manganese sulfate monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Manganese sulfate monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct

or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	100	0	152 862
Type B	0	44	6	202 034
Type C	0	0	0	236 067

The substance/substance group *Manganese sulfate monohydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9912 %)	88.0000 % (> 82.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24404	24404	0.00	207.71
26771	26771	0.00	232.83

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Mannitol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20118-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mannitol; Mannitolum

Special notes

When selecting the *Mannitol* substance/substance group, the following information is displayed to the user:

- Advice: The presence and absence of silica is not detectable by means of NIR. Please check the bulk density if necessary.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Mannitol	8	36	870

Second-stage model

For differentiation of the substance/substance group *Mannitol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Mannitol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	81.59	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Mannitol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Mannitol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Mannitol	12305723	20980	40	1402329
Caelo	Mannitol	15197305	22581	40	20150720
Euro OTC	Mannitol	1508012	21884	60	20150827*
Euro OTC	Mannitol	1511025	22286	60	20151228*
Euro OTC	Mannitol	2011022	25548	40	20210112*
Fagron	Mannitol	15A26-B01-305841	22883	40	20150204
Fagron	Mannitol	15A26-B01-305841	22884	40	20150204
Fagron	Mannitol	17B08-B04-352402	24579	40	20170517
Fagron	Mannitol	22D25-B04-224320	26396	40	20220629
Fagron	Mannitol	22D25-B04-224320	26396SI	20	20220629

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 420 spectra of 10 reference samples from the substance/substance group *Mannitol*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 542 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1670 spectra of 43 reference samples from the substance/substance group *Mannitol*.

- Among them are spectra of independent samples from 36 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Mannitol	160140	22458	60
Caelo	Mannitol	16014013	22580	40
Caelo	Mannitol	162009	22614	40
Caelo	Mannitol	162121	22721	40
Caelo	Mannitol	170879	23296	40
Caelo	Mannitol	170450	23318	40
Caelo	Mannitol	172588	23800	40
Caelo	Mannitol	182654	24368	40
Caelo	Mannitol	182655	24385	40
Caelo	Mannitol	191654	24723	40
Caelo	Mannitol	22001495	26249	40
Caelo	Mannitol	24000339	27137	40
Euro OTC	Mannitol	1604008	22515	40
Euro OTC	Mannitol	1606031	22697	40
Euro OTC	Mannitol	1610027	22862	40
Euro OTC	Mannitol	1703043	23125	40
Euro OTC	Mannitol	1708005	23700	40
Euro OTC	Mannitol	1802004	23966	40
Euro OTC	Mannitol	1806024	24152	40
Euro OTC	Mannitol	1809008	24327	40
Euro OTC	Mannitol	1902011	24476	40
Euro OTC	Mannitol	1904025	24600	40
Euro OTC	Mannitol	1908019	24857	40
Euro OTC	Mannitol	2004015	25161	40
Euro OTC	Mannitol	2008030	25323	40
Euro OTC	Mannitol	2105014	25678	40
Euro OTC	Mannitol	2108016	25822	50
Euro OTC	Mannitol	2108015	25826	50
Euro OTC	Mannitol	2108014	25828	50

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Mannitol	2201036	25957	40
Euro OTC	Mannitol	2205036	26218	40
Euro OTC	Mannitol	2209020	26343	40
Euro OTC	Mannitol	2301038	26598	40
Euro OTC	Mannitol	2307004	26858	40
Euro OTC	Mannitol	2401022	27149	40
Fagron	Mannitol	18H16-B01	24817	40
Caelo	Mannitol	162121	23066	30
Caelo	Mannitol	160140	23299	40
Caelo	Mannitol	170879	23305	40
Caelo	Mannitol	22001495	26249SI	20
Euro OTC	Mannitol	2201036	25957SI	10
Euro OTC	Mannitol	2205036	26218SI	20
Euro OTC	Mannitol	2209020	26343SI	20

- 200 414 spectra from a total of 4009 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3271 spectra from 824 *Apo-Ident* customers from 877 batches from the substance/substance group *Mannitol*.
- Among them are spectra of independent samples from 868 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Mannitol	20003605012	1
	Mannitol	21000744042	1
	Mannitol	21K16-B11-216336	2
	Mannitol	22001495005	2
	Mannitol	22001495015	7
	Mannitol	22001495017	3
	Mannitol	22001495019	1
	Mannitol	22001495023	3
	Mannitol	22001495041	1
	Mannitol	22001495046	1
	Mannitol	22001712003	1
	Mannitol	22001712004	2
	Mannitol	22001712008	5
	Mannitol	22001712009	1
	Mannitol	22001712010	1
	Mannitol	22001712011	7
	Mannitol	22001712012	2
	Mannitol	2201036-01	2
	Mannitol	2201495041	1
	Mannitol	2205036-01	3
	Mannitol	2209020-01	3
	Mannitol	22B22-F09	1
	Mannitol	22D25-B04-233814	1
	Mannitol	22E23-F15-38121	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Mannitol	22F15-F10-382723	1
	Mannitol	22F15-F15	2
	Mannitol	22F15-F20-382742	1
	Mannitol	2301038-01	2
	Mannitol	2307004-01	8
	Mannitol	2312007-01	2
	Mannitol	23A10-F03-384081	1
	Mannitol	23A10-F09	1
	Mannitol	23A10-F09-384083	1
	Mannitol	23A24F02-384302	1
	Mannitol	23A24-F02-384302	2
	Mannitol	23A24-F03-284303	1
	Mannitol	23A24-F03-38303	1
	Mannitol	23A24-F03-384303	2
	Mannitol	23A24-F05-384305	3
	Mannitol	23A24-F06-384306	1
	Mannitol	23A24-F07-384307	1
	Mannitol	23A24-F15-384487	2
	Mannitol	24000339007	4
	Mannitol	24000356001	2
	Mannitol	24000356002	3
	Mannitol	24000356003	3
	Mannitol	24000356005	1
	Mannitol	24000356007	2
	Mannitol	24000356010	1
AHC	Mannitol	18265511	1
AHC	Mannitol	20000958003	1
AHC	Mannitol	23I01-F01	1
AHD/EuRho02	Mannitol	1904025-02	1
AHD	Mannitol	2200195015	1
AHD	Mannitol	23A24-F04-384304	1
AHD	Mannitol	23A24-F05-384305	1
ALH/EuRho	Mannitol	1802004-01	1
ALH	Mannitol	1409016-01	1
ALH	Mannitol	1703043-01	1
Alliance / Fargon	Mannitol	19B12-B02-359604	1
Alliance Health 12.0...	Mannitol	1404034-01	2
Alliance Healthcare	Mannitol	18265409	1
Alliance Healthcare	Mannitol	2004015-01	1
alliance	Mannitol	2307004-01	1
Allianz Healthcare 2...	Mannitol	1502022-01	1
allianz	Mannitol	16212101	2
Anzag 05.10.17 8,04EUR	Mannitol	17045002	1
ANZAG	Mannitol	1211034-01	1
Anzag	Mannitol	1310004-02	1
Anzag	Mannitol	20003605007	3
Apo Ident/ Noweda	Mannitol	1610027-01	1
ApoIdent/Noweda	Mannitol	1610027-01	1
apomix	Mannitol	1310004-01	1
apomix	Mannitol	1708005-01	2
Bombastus	Mannitol	16340301	1
Cael Sanacorp 05.02.2016	Mannitol	14323138	2
Caeleo/ Kehr	Mannitol	182654001	1
Caelo	Mannitol		1
Caelo	Mannitol	10011501	1
Caelo	Mannitol	10100026	2
Caelo	Mannitol	1071701	1
Caelo	Mannitol	11(16200912)	1
Caelo	Mannitol	11003611	1
Caelo	Mannitol	1110009-02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Mannitol	11219121	1
Caelo	Mannitol	11219122	1
Caelo	Mannitol	11219124	2
Caelo	Mannitol	11308807	2
Caelo	Mannitol	11D01-N10	1
Caelo	Mannitol	1205016-01	2
Caelo	Mannitol	1205016-02	2
Caelo	Mannitol	12105403	3
Caelo	Mannitol	12105404	3
Caelo	Mannitol	12105405	1
Caelo	Mannitol	12105420	7
Caelo	Mannitol	12105421	9
Caelo	Mannitol	12105433	6
Caelo	Mannitol	12105438	2
Caelo	Mannitol	1211034-01	1
Caelo	Mannitol	12305709	16
Caelo	Mannitol	12305710	8
Caelo	Mannitol	12305723	4
Caelo	Mannitol	12305724	5
Caelo	Mannitol	12305725	11
Caelo	Mannitol	12305725-3444311112	1
Caelo	Mannitol	12305726	1
Caelo	Mannitol	12305728	2
Caelo	Mannitol	12305734	2
Caelo	Mannitol	12305736	4
Caelo	Mannitol	12305740	2
Caelo	Mannitol	1230578	1
Caelo	Mannitol	12411754	1
Caelo	Mannitol	1305043-02	3
Caelo	Mannitol	13095013	1
Caelo	Mannitol	1310004-01	3
Caelo	Mannitol	13189201	8
Caelo	Mannitol	13189203	8
Caelo	Mannitol	13189203-3566412081	1
Caelo	Mannitol	13189206	1
Caelo	Mannitol	13189207	8
Caelo	Mannitol	13189208	6
Caelo	Mannitol	13189215	17
Caelo	Mannitol	13189222	3
Caelo	Mannitol	13189226	4
Caelo	Mannitol	13189227	11
Caelo	Mannitol	13189228	1
Caelo	Mannitol	13K20-B01-287704	1
Caelo	Mannitol	14(20000685001)	1
Caelo	Mannitol	1400434-01	1
Caelo	Mannitol	1404034-01	2
Caelo	Mannitol	14051204	8
Caelo	Mannitol	14051205	7
Caelo	Mannitol	14051207	1
Caelo	Mannitol	14051208	2
Caelo	Mannitol	14051209	7
Caelo	Mannitol	14051215	7
Caelo	Mannitol	14051216	3
Caelo	Mannitol	14051217	2
Caelo	Mannitol	14051223	1
Caelo	Mannitol	14051224	2
Caelo	Mannitol	14051229	6
Caelo	Mannitol	14051230	2
Caelo	Mannitol	1405127	1
Caelo	Mannitol	1409016-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Mannitol	1423120	1
Caelo	Mannitol	14323101	3
Caelo	Mannitol	14323103	3
Caelo	Mannitol	14323105	2
Caelo	Mannitol	14323113	1
Caelo	Mannitol	14323114	3
Caelo	Mannitol	14323115	4
Caelo	Mannitol	14323120	1
Caelo	Mannitol	14323121	6
Caelo	Mannitol	14323124	2
Caelo	Mannitol	14323125	2
Caelo	Mannitol	14323126	4
Caelo	Mannitol	14323127	5
Caelo	Mannitol	14323129	1
Caelo	Mannitol	14323138	24
Caelo	Mannitol	14G04-B07-301693	2
Caelo	Mannitol	14g04-b07-30692	1
Caelo	Mannitol	1502022-01	1
Caelo	Mannitol	1508012-01	2
Caelo	Mannitol	1508012-02	1
Caelo	Mannitol	1511025-01	1
Caelo	Mannitol	151117	1
Caelo	Mannitol	15184101	1
Caelo	Mannitol	1519713	1
Caelo	Mannitol	15197219	1
Caelo	Mannitol	15197301	14
Caelo	Mannitol	15197302	5
Caelo	Mannitol	15197303	1
Caelo	Mannitol	15197312	1
Caelo	Mannitol	15197313	17
Caelo	Mannitol	15197314	6
Caelo	Mannitol	15197319	8
Caelo	Mannitol	15197327	1
Caelo	Mannitol	15197329	1
Caelo	Mannitol	15525	1
Caelo	Mannitol	15D28-B02-309192	4
Caelo	Mannitol	15K25-B04	1
Caelo	Mannitol	16011402	1
Caelo	Mannitol	16014005	12
Caelo	Mannitol	16014013	1
Caelo	Mannitol	16014014	1
Caelo	Mannitol	16014016	1
Caelo	Mannitol	160400801	2
Caelo	Mannitol	1606031-02	1
Caelo	Mannitol	16061401	1
Caelo	Mannitol	1610018-01	1
Caelo	Mannitol	1610027-01	3
Caelo	Mannitol	1612101	1
Caelo	Mannitol	16200901	2
Caelo	Mannitol	16200903	14
Caelo	Mannitol	16200904	2
Caelo	Mannitol	16200908	2
Caelo	Mannitol	16200909	1
Caelo	Mannitol	16200912	5
Caelo	Mannitol	16200913	4
Caelo	Mannitol	16200916	2
Caelo	Mannitol	16200924	11
Caelo	Mannitol	162121	1
Caelo	Mannitol	16212101	14
Caelo	Mannitol	16212102	15

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Mannitol	16212103	1
Caelo	Mannitol	16212104	2
Caelo	Mannitol	16212106	4
Caelo	Mannitol	16212109	4
Caelo	Mannitol	1621212	1
Caelo	Mannitol	16236603	1
Caelo	Mannitol	163403	1
Caelo	Mannitol	16340301	16
Caelo	Mannitol	16340302	7
Caelo	Mannitol	16D20-B03	1
Caelo	Mannitol	16F27-B05-324516	1
Caelo	Mannitol	16G27-B03	1
Caelo	Mannitol	16H25-B03-326639	1
Caelo	Mannitol	16H29-B05-327813	1
Caelo	Mannitol	16L15-B04-329317	1
Caelo	Mannitol	17/13-B03-340967	1
Caelo	Mannitol	17/13-B11	1
Caelo	Mannitol	1703043-01	1
Caelo	Mannitol	170450	1
Caelo	Mannitol	17045001	4
Caelo	Mannitol	17045002	19
Caelo	Mannitol	17045003	9
Caelo	Mannitol	17045004	3
Caelo	Mannitol	17045006	2
Caelo	Mannitol	17045008	7
Caelo	Mannitol	17045009	19
Caelo	Mannitol	17045010	5
Caelo	Mannitol	17050032/3	1
Caelo	Mannitol	170800501	3
Caelo	Mannitol	1708005-01	1
Caelo	Mannitol	17087907	1
Caelo	Mannitol	17087908	9
Caelo	Mannitol	17087909	3
Caelo	Mannitol	17087915	2
Caelo	Mannitol	17087916	21
Caelo	Mannitol	17258808	5
Caelo	Mannitol	17258809	11
Caelo	Mannitol	17258812	7
Caelo	Mannitol	17258819	5
Caelo	Mannitol	17258820	7
Caelo	Mannitol	17258823	3
Caelo	Mannitol	17258830	4
Caelo	Mannitol	17258830/P-09041922	1
Caelo	Mannitol	17258830/P-23051923	1
Caelo	Mannitol	17258831	4
Caelo	Mannitol	17260101	1
Caelo	Mannitol	17360101	20
Caelo	Mannitol	17360108	22
Caelo	Mannitol	17360110	5
Caelo	Mannitol	17360112	11
Caelo	Mannitol	17360114	1
Caelo	Mannitol	17360115	8
Caelo	Mannitol	17A12-B03	1
Caelo	Mannitol	17I13-B02-340966	1
Caelo	Mannitol	17j23-B05	1
Caelo	Mannitol	17J30B09343413	1
Caelo	Mannitol	17J30-B10-3434414	1
Caelo	Mannitol	17K29-B07-344253	1
Caelo	Mannitol	1802004-01	2
Caelo	Mannitol	180602401	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Mannitol	1806024-01	2
Caelo	Mannitol	1809008-01	3
Caelo	Mannitol	18121701	1
Caelo	Mannitol	1826504001	1
Caelo	Mannitol	182654001	1
Caelo	Mannitol	18265409	1
Caelo	Mannitol	18265410	5
Caelo	Mannitol	18265411	7
Caelo	Mannitol	18265417	3
Caelo	Mannitol	18265418	3
Caelo	Mannitol	18265427	1
Caelo	Mannitol	18265428	2
Caelo	Mannitol	18265429	1
Caelo	Mannitol	18265432	3
Caelo	Mannitol	18265436	2
Caelo	Mannitol	182655001	15
Caelo	Mannitol	182655002	1
Caelo	Mannitol	182655004	10
Caelo	Mannitol	18265502	15
Caelo	Mannitol	18265503	1
Caelo	Mannitol	18265504	5
Caelo	Mannitol	18265505	1
Caelo	Mannitol	18265506	17
Caelo	Mannitol	18265507	7
Caelo	Mannitol	18265508	11
Caelo	Mannitol	18265509	6
Caelo	Mannitol	18265511	12
Caelo	Mannitol	18265512	11
Caelo	Mannitol	18266513	1
Caelo	Mannitol	18A30-B03-346849	1
Caelo	Mannitol	18A30-B08	1
Caelo	Mannitol	18b23-b09	1
Caelo	Mannitol	18D09-B11-351436	1
Caelo	Mannitol	18D09-B12-351437	3
Caelo	Mannitol	18D09-B13-352214	2
Caelo	Mannitol	18D09-B14-352215	1
Caelo	Mannitol	18D09-B16-252503	1
Caelo	Mannitol	18e25-b07-352753	1
Caelo	Mannitol	19120-F15	1
Caelo	Mannitol	191654002	1
Caelo	Mannitol	191654003	2
Caelo	Mannitol	191654004	1
Caelo	Mannitol	19165401	6
Caelo	Mannitol	191654011	3
Caelo	Mannitol	191654012	1
Caelo	Mannitol	19165402	3
Caelo	Mannitol	19165403	1
Caelo	Mannitol	19165407	2
Caelo	Mannitol	19654002	1
Caelo	Mannitol	19J09-F07-366954	2
Caelo	Mannitol	19L19F14366950	1
Caelo	Mannitol	20000068507	1
Caelo	Mannitol	2000058001	1
Caelo	Mannitol	20000685001	7
Caelo	Mannitol	20000685006	2
Caelo	Mannitol	20000685007	2
Caelo	Mannitol	20000685008	1
Caelo	Mannitol	20000685012	15
Caelo	Mannitol	20000685013	3
Caelo	Mannitol	20000685014	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Mannitol	20000685017	1
Caelo	Mannitol	20000685021	1
Caelo	Mannitol	20000958001	11
Caelo	Mannitol	20000958003	7
Caelo	Mannitol	20000958006	7
Caelo	Mannitol	20000958007	6
Caelo	Mannitol	20001038003	1
Caelo	Mannitol	20002605010	1
Caelo	Mannitol	20003601002	1
Caelo	Mannitol	20003605002	8
Caelo	Mannitol	20003605003	1
Caelo	Mannitol	20003605004	12
Caelo	Mannitol	20003605006	1
Caelo	Mannitol	20003605007	11
Caelo	Mannitol	20003605008	5
Caelo	Mannitol	20003605010	9
Caelo	Mannitol	20003605011	2
Caelo	Mannitol	20003605013	9
Caelo	Mannitol	20003605015	5
Caelo	Mannitol	2000360510	2
Caelo	Mannitol	20003605504	1
Caelo	Mannitol	20004038002	1
Caelo	Mannitol	20004038003	5
Caelo	Mannitol	20004038004	2
Caelo	Mannitol	20004038006	1
Caelo	Mannitol	20004038007	5
Caelo	Mannitol	2000685006	1
Caelo	Mannitol	2000685014	1
Caelo	Mannitol	2000958003	1
Caelo	Mannitol	200218P302	1
Caelo	Mannitol	2003605007	1
Caelo	Mannitol	20151012-2	1
Caelo	Mannitol	20B05-F04-369845	1
Caelo	Mannitol	20H21F05373849	1
Caelo	Mannitol	21000744014	2
Caelo	Mannitol	21000744015	4
Caelo	Mannitol	21000744021	1
Caelo	Mannitol	21000744029	1
Caelo	Mannitol	21000744033	1
Caelo	Mannitol	21000744042	1
Caelo	Mannitol	2100074412	1
Caelo	Mannitol	2100074414	1
Caelo	Mannitol	2100342002	1
Caelo	Mannitol	21003432001	5
Caelo	Mannitol	21003432002	8
Caelo	Mannitol	2101401	1
Caelo	Mannitol	210501401	1
Caelo	Mannitol	2105014-01	1
Caelo	Mannitol	22001495002	2
Caelo	Mannitol	22001495009	1
Caelo	Mannitol	2200149501	1
Caelo	Mannitol	22001495016	2
Caelo	Mannitol	22001495017	1
Caelo	Mannitol	22001712001	2
Caelo	Mannitol	22001712003	3
Caelo	Mannitol	22001712004	3
Caelo	Mannitol	22001712007	1
Caelo	Mannitol	2274635	1
Caelo	Mannitol	23082013C	1
Caelo	Mannitol	24101306	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Mannitol	27101802	1
Caelo	Mannitol	30031502	1
Caelo	Mannitol	30121417	1
Caelo	Mannitol	4414E-01844	1
Caelo	Mannitol	4516E-01844	1
Caelo	Mannitol	48558	1
Caelo	Mannitol	5031304	1
Caelo	Mannitol	514E-01844	1
Caelo	Mannitol	7071404	1
Caelo	Mannitol	8031704	1
Caelo	Mannitol	8720	1
Caelo	Mannitol	9061808	1
Caelo	Mannitol	9081303	1
Caelo	Mannitol	9204719	1
Caelo	Mannitol	E911K	1
Caelo	Mannitol	E976E	1
Caesar & Lorenz GmbH	Mannitol	18265507	1
Caesar & Loretz GmbH...	Mannitol	16200908	1
Caesar & Loretz GmbH...	Mannitol	18265509	1
Caesar & Loretz GmbH...	Mannitol	21000744006	1
Caesar & Loretz GmbH...	Mannitol	17258819	1
Caesar & Loretz GmbH/AHD	Mannitol	20003605011	1
Caesar & Loretz GmbH/GEHE	Mannitol	182655001	1
Caesar & Loretz GmbH/GEHE	Mannitol	20000958003	1
Caesar & Loretz GmbH/GEHE	Mannitol	20000958007	1
Caesar & Loretz GmbH/GEHE	Mannitol	20003605002	2
Caesar & Loretz GmbH...	Mannitol	191654004	1
Caesar & Loretz GmbH...	Mannitol	20000685007	4
Caesar & Loretz GmbH...	Mannitol	20004038004	2
Caesar & Loretz GmbH...	Mannitol	18265509	1
Caesar & Loretz GmbH...	Mannitol	18265512	1
Caesar & Loretz GmbH/Kehr	Mannitol	182655001	1
Caesar & Loretz GmbH/Kehr	Mannitol	18265508	1
Caesar & Loretz GmbH...	Mannitol	18265432	3
Caesar & Loretz GmbH...	Mannitol	17258809	1
Caesar & Loretz GmbH...	Mannitol	18265511	2
Caesar & Loretz GmbH/Phö	Mannitol	20000958003	1
Caesar & Loretz GmbH/Phoe	Mannitol	20003605007	1
Caesar & Loretz GmbH...	Mannitol	20003605012	1
Caesar & Loretz GmbH...	Mannitol	22001712004	14
Caesar & Loretz GmbH...	Mannitol	20000685014	1
Caesar & Loretz GmbH...	Mannitol	20003605002	1
Caesar & Loretz GmbH/Sana	Mannitol	20003605002	1
Caesar & Loretz GmbH...	Mannitol	2000058001	1
Caesar & Loretz GmbH	Mannitol	13189207	1
Caesar & Loretz GmbH	Mannitol	14323119	1
Caesar & Loretz GmbH	Mannitol	17087915	1
Caesar & Loretz GmbH	Mannitol	17258809	2
Caesar & Loretz GmbH	Mannitol	17258819	1
Caesar & Loretz GmbH	Mannitol	17258820	1
Caesar & Loretz GmbH	Mannitol	17360112	1
Caesar & Loretz GmbH	Mannitol	17360114	2
Caesar & Loretz GmbH	Mannitol	1826508	1
Caesar & Loretz GmbH	Mannitol	18265408	2
Caesar & Loretz GmbH	Mannitol	18265409	1
Caesar & Loretz GmbH	Mannitol	18265417	3
Caesar & Loretz GmbH	Mannitol	18265418	2
Caesar & Loretz GmbH	Mannitol	18265420	5
Caesar & Loretz GmbH	Mannitol	18265431	1
Caesar & Loretz GmbH	Mannitol	182655001	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Mannitol	182655002	5
Caesar & Loretz GmbH	Mannitol	182655004	2
Caesar & Loretz GmbH	Mannitol	18265502	3
Caesar & Loretz GmbH	Mannitol	18265503	2
Caesar & Loretz GmbH	Mannitol	18265504	7
Caesar & Loretz GmbH	Mannitol	18265505	4
Caesar & Loretz GmbH	Mannitol	18265506	3
Caesar & Loretz GmbH	Mannitol	18265507	1
Caesar & Loretz GmbH	Mannitol	18265508	10
Caesar & Loretz GmbH	Mannitol	18265509	1
Caesar & Loretz GmbH	Mannitol	18265510	1
Caesar & Loretz GmbH	Mannitol	18265511	4
Caesar & Loretz GmbH	Mannitol	18265512	2
Caesar & Loretz GmbH	Mannitol	191654004	3
Caesar & Loretz GmbH	Mannitol	19165401	3
Caesar & Loretz GmbH	Mannitol	191654012	1
Caesar & Loretz GmbH	Mannitol	20000685001	3
Caesar & Loretz GmbH	Mannitol	20000685007	1
Caesar & Loretz GmbH	Mannitol	20000958001	5
Caesar & Loretz GmbH	Mannitol	20000958003	2
Caesar & Loretz GmbH	Mannitol	20000958006	1
Caesar & Loretz GmbH	Mannitol	20000958007	6
Caesar & Loretz GmbH	Mannitol	20003605002	3
Caesar & Loretz GmbH	Mannitol	20003605004	3
Caesar & Loretz GmbH	Mannitol	20003605006	1
Caesar & Loretz GmbH	Mannitol	20003605007	2
Caesar & Loretz GmbH	Mannitol	20003605008	1
Caesar & Loretz GmbH	Mannitol	20003605010	2
Caesar & Loretz GmbH	Mannitol	20003605012	2
Caesar & Loretz GmbH	Mannitol	20003605013	2
Caesar & Loretz GmbH	Mannitol	20004038004	3
Caesar & Loretz GmbH	Mannitol	21000744014	2
Caesar & Loretz GmbH	Mannitol	21000744029	4
Caesar & Loretz GmbH	Mannitol	21000744042	2
Caesar & Loretz GmbH	Mannitol	21003432001	2
Caesar & Loretz GmbH	Mannitol	21003432002	2
Caesar & Loretz GmbH	Mannitol	22001495002	1
Caesar & Loretz GmbH	Mannitol	22001495006	5
Caesar & Loretz GmbH	Mannitol	22001495017	1
Caesar & Loretz GmbH	Mannitol	22001712001	1
Caesar & Loretz GmbH	Mannitol	22001712003	1
Caesar & Loretz GmbH	Mannitol	22001712004	4
Caesar & Loretz GmbH	Mannitol	22001712006	1
Caesar & Loretz GmbH	Mannitol	22001712007	1
Caesar & Loretz/Noweda	Mannitol	182655004	1
Caesar & Loretz/Noweda	Mannitol	20003605004	1
Caesar & Loretz/Noweda	Mannitol	20003605007	1
Caesar/Ebert	Mannitol	17360108	1
Caesar	Mannitol	1508012-1	1
Caleo/ Noweda	Mannitol	18J04-B05-355467	1
Calo/Noweda	Mannitol	23A10-F13-384084	1
ceal	Mannitol	17045006	1
Cealo, Noweda	Mannitol	20003605002	1
Cealo/Gehe	Mannitol	18265502	1
cealo/phoenix	Mannitol	14323138	2
Celo/Phoenix	Mannitol	20003605004	1
Celo	Mannitol	15197313	1
cesar&lorentz/Phönix	Mannitol	12305710	1
Defektur/eigen	Mannitol	1604008-01	1
Delta	Mannitol	1610027-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Ebert & Jacobi	Mannitol	12305728	1
EuRho Pharma	Mannitol	1704010-01	1
EuRho/GEHE	Mannitol	1409016-01	1
EuRho/GEHE	Mannitol	1409016-02	1
EuRho/Gehe	Mannitol	1802004-01	1
EuRho/Noweda	Mannitol	1703043-01	1
EuRho/Noweda	Mannitol	1806024-01	1
EuRho/Noweda	Mannitol	1904025-01	2
EuRho/Phoenix	Mannitol	1508012-01	1
EuRho/Sanac	Mannitol	1305043-01	1
EuRho	Mannitol	1205016-01	1
EuRho	Mannitol	1211034-01	1
EuRho	Mannitol	1211034-02	1
EuRho	Mannitol	1404034-01	1
EuRho	Mannitol	1404034-02	2
EuRho	Mannitol	1502022-02	1
EuRho	Mannitol	1508012-01	7
EuRho	Mannitol	1511025-01	1
EuRho	Mannitol	1911M-01844	1
EuRho	Mannitol	2108016-01	1
Eurho	Mannitol	2201036-01	2
EuRhoPha	Mannitol	1404034-01	1
Euro OTC	Mannitol	1006019-01	1
Euro OTC	Mannitol	10112014E	1
Euro OTC	Mannitol	1104028-01	1
Euro OTC	Mannitol	1104028-03	3
Euro OTC	Mannitol	1110009-01	10
Euro OTC	Mannitol	1110009-02	4
Euro OTC	Mannitol	111100009-02	1
Euro OTC	Mannitol	1205016	1
Euro OTC	Mannitol	1205016-01	11
Euro OTC	Mannitol	1205016-02	2
Euro OTC	Mannitol	12105433	3
Euro OTC	Mannitol	1211034-01	9
Euro OTC	Mannitol	1211034-02	14
Euro OTC	Mannitol	1305043	1
Euro OTC	Mannitol	130504301	1
Euro OTC	Mannitol	1305043-01	12
Euro OTC	Mannitol	1305043-02	14
Euro OTC	Mannitol	1310004-01	14
Euro OTC	Mannitol	1310004-02	8
Euro OTC	Mannitol	13155710	1
Euro OTC	Mannitol	13189216	2
Euro OTC	Mannitol	14003402	1
Euro OTC	Mannitol	140403401	1
Euro OTC	Mannitol	1404034-01	15
Euro OTC	Mannitol	140403402	2
Euro OTC	Mannitol	1404034-02	16
Euro OTC	Mannitol	1404036-02	1
Euro OTC	Mannitol	1409016-01	19
Euro OTC	Mannitol	1409016-02	6
Euro OTC	Mannitol	1409016-1	1
Euro OTC	Mannitol	15002022-01	1
Euro OTC	Mannitol	1502022/01	1
Euro OTC	Mannitol	150202201	2
Euro OTC	Mannitol	1502022-01	17
Euro OTC	Mannitol	150202202	1
Euro OTC	Mannitol	1502022-02	5
Euro OTC	Mannitol	150801	1
Euro OTC	Mannitol	150801201	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Mannitol	1508012-01	33
Euro OTC	Mannitol	1508012-02	14
Euro OTC	Mannitol	150916M	1
Euro OTC	Mannitol	1511024-01	1
Euro OTC	Mannitol	151102501	2
Euro OTC	Mannitol	1511025-01	42
Euro OTC	Mannitol	151105-01	1
Euro OTC	Mannitol	158012-01	1
Euro OTC	Mannitol	160027-01	1
Euro OTC	Mannitol	16006031-01	1
Euro OTC	Mannitol	160400	2
Euro OTC	Mannitol	16040008-01	1
Euro OTC	Mannitol	1604002-01	1
Euro OTC	Mannitol	1604008	1
Euro OTC	Mannitol	160400801	1
Euro OTC	Mannitol	1604008-01	44
Euro OTC	Mannitol	160408-01	1
Euro OTC	Mannitol	160601-01	1
Euro OTC	Mannitol	160603101	1
Euro OTC	Mannitol	1606031-01	24
Euro OTC	Mannitol	1606031-02	8
Euro OTC	Mannitol	161002701	3
Euro OTC	Mannitol	1610027-01	34
Euro OTC	Mannitol	1610027-02	2
Euro OTC	Mannitol	1610027-1	1
Euro OTC	Mannitol	161129M/1604008-01	1
Euro OTC	Mannitol	16D20-B04-320487	1
Euro OTC	Mannitol	16H29-B02	1
Euro OTC	Mannitol	17/14	1
Euro OTC	Mannitol	170304301	3
Euro OTC	Mannitol	1703043-01	16
Euro OTC	Mannitol	170304302	1
Euro OTC	Mannitol	1703043-02	11
Euro OTC	Mannitol	1703049-01	1
Euro OTC	Mannitol	1704010-01	6
Euro OTC	Mannitol	1704010-10	1
Euro OTC	Mannitol	1708005	1
Euro OTC	Mannitol	170800501	1
Euro OTC	Mannitol	1708005-01	42
Euro OTC	Mannitol	1708005-02	4
Euro OTC	Mannitol	1708005-05	1
Euro OTC	Mannitol	17087908	1
Euro OTC	Mannitol	178005-01	1
Euro OTC	Mannitol	180200401	2
Euro OTC	Mannitol	1802004-01	30
Euro OTC	Mannitol	180219M/1708005-01	1
Euro OTC	Mannitol	1806024/01	1
Euro OTC	Mannitol	180602401	1
Euro OTC	Mannitol	1806024-01	22
Euro OTC	Mannitol	1806024-1	1
Euro OTC	Mannitol	180624-01	2
Euro OTC	Mannitol	1809008-001	1
Euro OTC	Mannitol	1809008-002	1
Euro OTC	Mannitol	1809008-01	32
Euro OTC	Mannitol	180900802	1
Euro OTC	Mannitol	1809008-02	19
Euro OTC	Mannitol	1901092	2
Euro OTC	Mannitol	1902011-01	20
Euro OTC	Mannitol	1904023-03	1
Euro OTC	Mannitol	1904025	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Mannitol	190402501	1
Euro OTC	Mannitol	1904025-01	16
Euro OTC	Mannitol	190402502	1
Euro OTC	Mannitol	1904025-02	44
Euro OTC	Mannitol	1904025-03	19
Euro OTC	Mannitol	1904025-12	1
Euro OTC	Mannitol	190801901	1
Euro OTC	Mannitol	1908019-01	1
Euro OTC	Mannitol	1908019-02	5
Euro OTC	Mannitol	19I20-F12	1
Euro OTC	Mannitol	200401501	1
Euro OTC	Mannitol	2004015-01	32
Euro OTC	Mannitol	200803001	1
Euro OTC	Mannitol	2008030-01	32
Euro OTC	Mannitol	2011022-01	16
Euro OTC	Mannitol	2011022-011	1
Euro OTC	Mannitol	204015-01	1
Euro OTC	Mannitol	20B05-F03-369844	1
Euro OTC	Mannitol	2105014-01	15
Euro OTC	Mannitol	2108014-01	4
Euro OTC	Mannitol	2108015-01	6
Euro OTC	Mannitol	2108016-01	5
Euro OTC	Mannitol	2201036_01	1
Euro OTC	Mannitol	2201036-01	11
Euro OTC	Mannitol	2205036	1
Euro OTC	Mannitol	2205036-01	7
Euro OTC	Mannitol	2209020-01	9
Euro OTC	Mannitol	2301038-01	2
Euro OTC	Mannitol	E112N	2
Euro OTC	Mannitol	e118t	1
Euro OTC	Mannitol	E118T	3
Euro OTC	Mannitol	E224X	1
Euro OTC	Mannitol	E235L	1
Euro OTC	Mannitol	E312J	1
Euro OTC	Mannitol	E331X	1
Euro OTC	Mannitol	E671Z	1
Euro OTC	Mannitol	E976E	2
Euro OTC	Mannitol	T03-07/1409016-01	1
Euro/Gehe	Mannitol	1508012-01	2
Euro/Noweda	Mannitol	1902011-01	2
Euro/Phönix	Mannitol	1904025-02	1
EURO	Mannitol	170401001	1
EurpTec/ Alliance He…	Mannitol	1610027-02	1
Fagon	Mannitol	13K20-B01-292064	1
Fagron	Mannitol		1
Fagron	Mannitol	10974140	1
Fagron	Mannitol	11219122	1
Fagron	Mannitol	11L19-N15	1
Fagron	Mannitol	12E24-N03	1
Fagron	Mannitol	12J26-N15	1
Fagron	Mannitol	12K28-N01	1
Fagron	Mannitol	1302C004	2
Fagron	Mannitol	1302C005	1
Fagron	Mannitol	13B01-B05-283812	1
Fagron	Mannitol	13E24N01	1
Fagron	Mannitol	13K20-B01	1
Fagron	Mannitol	13K20-B01-287698	2
Fagron	Mannitol	13K20-B01-287706	1
Fagron	Mannitol	13K20-B01-294193	1
Fagron	Mannitol	13K20-B01-294194	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Mannitol	14323121	1
Fagron	Mannitol	14G004-B07-301692	1
Fagron	Mannitol	14G04-B07	4
Fagron	Mannitol	14G04-B07-296196	1
Fagron	Mannitol	14G04-B07-301685	1
Fagron	Mannitol	14G04-B07-301692	15
Fagron	Mannitol	14G04-B07-301693	1
Fagron	Mannitol	14G04-B07-301694	1
Fagron	Mannitol	14G17-B06-301921	1
Fagron	Mannitol	1502022-01	3
Fagron	Mannitol	15A26-B01-304717	4
Fagron	Mannitol	15B05-B04-304084	4
Fagron	Mannitol	15B05-B05-304085	1
Fagron	Mannitol	15C04-B04-311796	1
Fagron	Mannitol	15D28-B02-309192	4
Fagron	Mannitol	15D28-B02-309193	1
Fagron	Mannitol	15I24-B04	1
Fagron	Mannitol	15K17-B01-315560	3
Fagron	Mannitol	15K17-B03-314903	1
Fagron	Mannitol	15K25-B04-317786	2
Fagron	Mannitol	15K25-B06-318740	3
Fagron	Mannitol	16/28-B01-328593	1
Fagron	Mannitol	16212103	1
Fagron	Mannitol	16340301	1
Fagron	Mannitol	16B24-B09-32001	1
Fagron	Mannitol	16B24-B09-320013	2
Fagron	Mannitol	16D20-B03	1
Fagron	Mannitol	16D20-B03-320486	1
Fagron	Mannitol	16D20-B04-320487	1
Fagron	Mannitol	16E11-B04	1
Fagron	Mannitol	16E11-B06	1
Fagron	Mannitol	16E11B07322830	1
Fagron	Mannitol	16E11-B07-322830	2
Fagron	Mannitol	16E11-B08	1
Fagron	Mannitol	16E11-B08-323540	1
Fagron	Mannitol	16F01-B03-322189	1
Fagron	Mannitol	16F27-B04-32483	1
Fagron	Mannitol	16F27-B05-324516	2
Fagron	Mannitol	16G27-B03	1
Fagron	Mannitol	16G27-B03-324517	1
Fagron	Mannitol	16G27-B05-325659	2
Fagron	Mannitol	16H02-B01-325660	1
Fagron	Mannitol	16H25-B03-326639	3
Fagron	Mannitol	16H29-B02-326640	2
Fagron	Mannitol	16H29-B03-326641	1
Fagron	Mannitol	16H29-B05-327813	2
Fagron	Mannitol	16J28-B01-328593	2
Fagron	Mannitol	16L15-B04	1
Fagron	Mannitol	16L15-B04-329317	2
Fagron	Mannitol	16L15-B05-329316	1
Fagron	Mannitol	17/13-B04-340968	3
Fagron	Mannitol	17/13-B10	1
Fagron	Mannitol	17/13-B11-341331	1
Fagron	Mannitol	17045002	1
Fagron	Mannitol	170612185	1
Fagron	Mannitol	17123B05342007	1
Fagron	Mannitol	1713-B11	1
Fagron	Mannitol	17A12-B02	1
Fagron	Mannitol	17A12-B02-332068	2
Fagron	Mannitol	17A12-B03	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Mannitol	17A12-B04-330729	1
Fagron	Mannitol	17A12-Bo3	1
Fagron	Mannitol	17A27-B02	1
Fagron	Mannitol	17A27-B02-331292	4
Fagron	Mannitol	17B08-B02	2
Fagron	Mannitol	17B08-B04	3
Fagron	Mannitol	17B08-B04_352402	1
Fagron	Mannitol	17B08-B04-334312	2
Fagron	Mannitol	17B08-B04-334313	1
Fagron	Mannitol	17B08-B04-334314	1
Fagron	Mannitol	17B08-B04-352402	5
Fagron	Mannitol	17C28-B03-333349	1
Fagron	Mannitol	17C28-B05333613	1
Fagron	Mannitol	17C28-B06	2
Fagron	Mannitol	17D12-B01-334435	6
Fagron	Mannitol	17D18-B01	1
Fagron	Mannitol	17D18-B03-335437	2
Fagron	Mannitol	17E03-B01-336748	1
Fagron	Mannitol	17F27-B03-337911	1
Fagron	Mannitol	17F27B04337912	1
Fagron	Mannitol	17F27B04-337912	1
Fagron	Mannitol	17F27-B04-337912	2
Fagron	Mannitol	17F27-B05-337913	1
Fagron	Mannitol	17F27-B07	2
Fagron	Mannitol	17F27-B07-338598	2
Fagron	Mannitol	17F27-B08	1
Fagron	Mannitol	17F27-B08-338599	1
Fagron	Mannitol	17I13B03340967	1
Fagron	Mannitol	17I13-B03-340967	2
Fagron	Mannitol	17I13-B04-340968	1
Fagron	Mannitol	17I13-B10	1
Fagron	Mannitol	17I13-B11-341331	1
Fagron	Mannitol	17J04-B06	1
Fagron	Mannitol	17J04-B06-341798	2
Fagron	Mannitol	17J04-B07-341800	1
Fagron	Mannitol	17J23-B05	2
Fagron	Mannitol	17J23-B05-342007	4
Fagron	Mannitol	17J23-B06	1
Fagron	Mannitol	17J30309-343413	1
Fagron	Mannitol	17J30-B09-343413	2
Fagron	Mannitol	17J30-B10-343414	2
Fagron	Mannitol	17J30-B11-343939	1
Fagron	Mannitol	17K29-B04-343940	1
Fagron	Mannitol	17K29-B05	1
Fagron	Mannitol	17K29-B05-345229	3
Fagron	Mannitol	17K29-B07-344253	1
Fagron	Mannitol	17L04-B03-345230	1
Fagron	Mannitol	17L04-B04-345231	2
Fagron	Mannitol	17L18-B04-351506	1
Fagron	Mannitol	17LO4-B08	1
Fagron	Mannitol	18/25-B08-356984	2
Fagron	Mannitol	1806024-01	1
Fagron	Mannitol	1830-08-346849	1
Fagron	Mannitol	18A30-B06-346848	3
Fagron	Mannitol	18A30-B07-348872	3
Fagron	Mannitol	18A30-B08-346849	3
Fagron	Mannitol	18A30-B09-346850	1
Fagron	Mannitol	18A30-B10	1
Fagron	Mannitol	18B23-B10-349553	3
Fagron	Mannitol	18B23-B12-349972	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Mannitol	18D09-B11	1
Fagron	Mannitol	18D09-B11-351436	3
Fagron	Mannitol	18D09-B13	1
Fagron	Mannitol	18D09-B13-352214	2
Fagron	Mannitol	18D09-B15-352216	1
Fagron	Mannitol	18D09-B16-352503	1
Fagron	Mannitol	18E25-B05-352504	2
Fagron	Mannitol	18E25-B06-352505	2
Fagron	Mannitol	18E25-B07	1
Fagron	Mannitol	18E25-B07-352753	1
Fagron	Mannitol	18E25-B-07-352753	1
Fagron	Mannitol	18E25-B08	1
Fagron	Mannitol	18E25-B08-352754	1
Fagron	Mannitol	18E25B09352755	1
Fagron	Mannitol	18E25-B09-352755	4
Fagron	Mannitol	18g04-813-3541621	1
Fagron	Mannitol	18G04-B09	1
Fagron	Mannitol	18G04-B10-354321	2
Fagron	Mannitol	18G04-B11-354322	1
Fagron	Mannitol	18G04-B13	2
Fagron	Mannitol	18G04-B13-354621	6
Fagron	Mannitol	18H16-B01-357217	2
Fagron	Mannitol	18H16-B01-359311	1
Fagron	Mannitol	18H16-B01-3633309	1
Fagron	Mannitol	18H16-B01-365268	1
Fagron	Mannitol	18J04-B05-355467	4
Fagron	Mannitol	18j04B07-355587	1
Fagron	Mannitol	18J04-B07-355587	1
Fagron	Mannitol	18J04-B10-355589	1
Fagron	Mannitol	18J25-B05-356984	1
Fagron	Mannitol	18J25-B07-356983	1
Fagron	Mannitol	18J25-B08	1
Fagron	Mannitol	18J25-B08-356984	3
Fagron	Mannitol	18L03-B03	3
Fagron	Mannitol	18L03-B03-357463	2
Fagron	Mannitol	18L03-B06-357782	1
Fagron	Mannitol	18L21-B03	1
Fagron	Mannitol	18L21-B03-358869	1
Fagron	Mannitol	18L21-B04-358870	2
Fagron	Mannitol	18L21-B04-358879	1
Fagron	Mannitol	18L21-B05	1
Fagron	Mannitol	18L21-B05-358871	5
Fagron	Mannitol	18L21-B06-3558872	1
Fagron	Mannitol	18L21-B06-358872	1
Fagron	Mannitol	18L21-B08-358874	1
Fagron	Mannitol	19/19-F10-366892	1
Fagron	Mannitol	19/20-F07-366390	1
Fagron	Mannitol	19/20-F12-366393	1
Fagron	Mannitol	19120-F09-366392	1
Fagron	Mannitol	19120F13366394	1
Fagron	Mannitol	19120-F15-366395	1
Fagron	Mannitol	19A14-B03-360504	2
Fagron	Mannitol	19A14-B04_360505	1
Fagron	Mannitol	19A14B04360505	1
Fagron	Mannitol	19A14-B04-360505	4
Fagron	Mannitol	19A14-B05-360506	1
Fagron	Mannitol	19A14-B06-360507	1
Fagron	Mannitol	19B12-B02	2
Fagron	Mannitol	19B12-B02-359604	1
Fagron	Mannitol	19B12-B03-059605	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Mannitol	19B12-B03-359605	1
Fagron	Mannitol	19C11B02361201	1
Fagron	Mannitol	19C11B02-361201	1
Fagron	Mannitol	19C11-B02-361201	2
Fagron	Mannitol	19C11-B03-361202	1
Fagron	Mannitol	19C11B04361203	1
Fagron	Mannitol	19C11-B04-361203	1
Fagron	Mannitol	19C11-B05-361204	1
Fagron	Mannitol	19C14-B02-361206	1
Fagron	Mannitol	19C14-B06321213	1
Fagron	Mannitol	19c14-B06-361213	1
Fagron	Mannitol	19D16-B03	1
Fagron	Mannitol	19D16-B03-364401	3
Fagron	Mannitol	19D16-B04-364402	1
Fagron	Mannitol	19D16-B05	1
Fagron	Mannitol	19E06-B05-363487	3
Fagron	Mannitol	19E06B06363488	1
Fagron	Mannitol	19E06-B06-363488	6
Fagron	Mannitol	19E06-B08-363490	1
Fagron	Mannitol	19F12-B09-363871	3
Fagron	Mannitol	19F12-B10-363872	3
Fagron	Mannitol	19F12-B11	1
Fagron	Mannitol	19F12-b11-363873	1
Fagron	Mannitol	19F12-B11-363873	1
Fagron	Mannitol	19I19-F1	1
Fagron	Mannitol	19I19-F10	1
Fagron	Mannitol	19I19-F10-366892	3
Fagron	Mannitol	19I19-F11-366893	1
Fagron	Mannitol	19I19-F14-366950	2
Fagron	Mannitol	19I20_F13-366394	1
Fagron	Mannitol	19I20-F09	1
Fagron	Mannitol	19I20-F09-366392	1
Fagron	Mannitol	19I20-F12-366393	2
Fagron	Mannitol	19I20-F13	1
Fagron	Mannitol	19i20-f15	1
Fagron	Mannitol	19I20-F15	1
Fagron	Mannitol	19I20-F15-366395	4
Fagron	Mannitol	19J09-F03	1
Fagron	Mannitol	19J09-F08-366955	2
Fagron	Mannitol	20006F20375113	1
Fagron	Mannitol	20B05-04-369845	1
Fagron	Mannitol	20B05-F03	3
Fagron	Mannitol	20B05-F04	1
Fagron	Mannitol	20B05F04369845	2
Fagron	Mannitol	20B05-F05-369846	1
Fagron	Mannitol	20B05-F06	1
Fagron	Mannitol	20B05-F06-369847	1
Fagron	Mannitol	20C06-F06	1
Fagron	Mannitol	20C06-F06-369853	1
Fagron	Mannitol	20C06-F07-369854	1
Fagron	Mannitol	20D16F11	1
Fagron	Mannitol	20D16-F11-371552	2
Fagron	Mannitol	20D16-F12	2
Fagron	Mannitol	20D16-F12-371553	4
Fagron	Mannitol	20D16-F13-371555	5
Fagron	Mannitol	20D16F14371554	1
Fagron	Mannitol	20D16-F15	1
Fagron	Mannitol	20E25-F06-372224	1
Fagron	Mannitol	20E25-F07-372221	5
Fagron	Mannitol	20E25-F08-372222	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Mannitol	20F12_F06_373767	1
Fagron	Mannitol	20F12-F06-373767	3
Fagron	Mannitol	20F12-F07	1
Fagron	Mannitol	20F12-F07-373768	2
Fagron	Mannitol	20F12-F08	2
Fagron	Mannitol	20F12-F08-373769	1
Fagron	Mannitol	20F12-F09-373770	3
Fagron	Mannitol	20F12-F10-373771	2
Fagron	Mannitol	20F12-F15-373776	1
Fagron	Mannitol	20F12-F-373768	1
Fagron	Mannitol	20H21-06	1
Fagron	Mannitol	20H21-F03	1
Fagron	Mannitol	20H21-F03-373847	3
Fagron	Mannitol	20H21-F04-373848	5
Fagron	Mannitol	20H21-F05-373849	1
Fagron	Mannitol	20H21-F06-373987	5
Fagron	Mannitol	20H21-F08-373989	2
Fagron	Mannitol	20H21-F09	1
Fagron	Mannitol	20H21-F09-373990	1
Fagron	Mannitol	20J06F13	1
Fagron	Mannitol	20J06-F13	1
Fagron	Mannitol	20J06-F14-375107	2
Fagron	Mannitol	20J06-F15-375108	3
Fagron	Mannitol	20J06-F16	2
Fagron	Mannitol	20J06-F21-375114	2
Fagron	Mannitol	20L1115-F10-376720	1
Fagron	Mannitol	20L15-F10	1
Fagron	Mannitol	20L15-F10-376720	2
Fagron	Mannitol	20L15-F15-376869	2
Fagron	Mannitol	21B12F04377243	1
Fagron	Mannitol	21B12-F04-377243	3
Fagron	Mannitol	21C31-F04-378222	4
Fagron	Mannitol	21C31-F06	1
Fagron	Mannitol	21C31F04	1
Fagron	Mannitol	21D02F05	1
Fagron	Mannitol	21D02-F05	1
Fagron	Mannitol	21D02-F06-378226	4
Fagron	Mannitol	21E25-F07	1
Fagron	Mannitol	21E25f07-379700	1
Fagron	Mannitol	21E25-F07-379700	2
Fagron	Mannitol	21E25-F08-379701	3
Fagron	Mannitol	21f16f05379703	1
Fagron	Mannitol	21H04-F05	3
Fagron	Mannitol	21H04-F05-379996	1
Fagron	Mannitol	21K10-F01-380693	1
Fagron	Mannitol	21K10-F04	2
Fagron	Mannitol	21K16-B11-216336	2
Fagron	Mannitol	22822F-06	1
Fagron	Mannitol	22A12-F05-381468	2
Fagron	Mannitol	22A12-F07-381470	2
Fagron	Mannitol	22A12-F09-381478	1
Fagron	Mannitol	22A12-F14	1
Fagron	Mannitol	22A12-F14-381239	3
Fagron	Mannitol	22B01-F04	1
Fagron	Mannitol	22B01-F04-381542	2
Fagron	Mannitol	22B22-F06-381606	5
Fagron	Mannitol	22B22F08	1
Fagron	Mannitol	22B22-F08-381608	2
Fagron	Mannitol	22B22-F13	1
Fagron	Mannitol	22B22-F13-381720	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Mannitol	22B22-F14-381721	1
Fagron	Mannitol	22B22-F15	1
Fagron	Mannitol	22B22-F15-381722	4
Fagron	Mannitol	22e23f12	1
Fagron	Mannitol	22E23-F12-382118	1
Fagron	Mannitol	22E23-F13-382119	3
Fagron	Mannitol	22E23-F14	3
Fagron	Mannitol	22E23-F14-382120	3
Fagron	Mannitol	22E23-F15	2
Fagron	Mannitol	22E23-F15-382121	1
Fagron	Mannitol	22E23-F17-382114	1
Fagron	Mannitol	22E23F18382115	1
Fagron	Mannitol	22E23-F19-382117	5
Fagron	Mannitol	22E23-F21-382116	2
Fagron	Mannitol	22E23F-F06	1
Fagron	Mannitol	22F15-F10-382723	1
Fagron	Mannitol	22F15-F12-382724	1
Fagron	Mannitol	22F15F15382727	1
Fagron	Mannitol	22F15-F15-382727	1
Fagron	Mannitol	22F15F16382728	1
Fagron	Mannitol	22F15-F17-382731	1
Fagron	Mannitol	22F15-F18-382732	1
Fagron	Mannitol	22F15-F20	1
Fagron	Mannitol	22F15-F20-382742	2
Fagron	Mannitol	23A10_F03_384081	1
Fagron	Mannitol	23A10-F07-384082	1
Fagron	Mannitol	23A10-F09-384083	2
Fagron	Mannitol	23A10-F09-384303	1
Fagron	Mannitol	23A10-F14-384085	1
Fagron	Mannitol	23a24-f03-384303	1
Fagron	Mannitol	23A24-F13-384485	1
Fagron	Mannitol	296196	1
Fagron	Mannitol	4092019Mi	1
Fagron	Mannitol	5-37970003	1
Fagron	Mannitol	6E11-B08-323540	1
Fagron	Mannitol	720014-0001	2
Fagron	Mannitol	720014-0002	1
Fagron	Mannitol	B04-3524002	1
Fagron	Mannitol	E166K/21K16-B11-216336	1
Fagron	Mannitol	E611X	1
Fagron	Mannitol	E833Z	1
Fagron	Mannitol	E911K	1
Fagron	Mannitol	f07-3814700	1
Fagron	Mannitol	F08-3737609	1
Fagron	Mannitol	F09-3737700	1
Fagrron	Mannitol	17C28-B05-33361	1
Fargon - Alliance He…	Mannitol	19I20-F13-366394	1
Fargon / Noweda	Mannitol	20J06-F20	1
Fargon/ Noweda	Mannitol	15A26-B01-304717	1
Fargon/ Phoenix	Mannitol	19I20-F13-366394	1
Fargon/Noweda	Mannitol	19016-B03	1
Fargon	Mannitol	12E24-N08	1
Fargon	Mannitol	18B23-B10-349553	1
Fargon	Mannitol	18D09-B16-352503	1
Fiebig/Farago	Mannitol	19E06-B06-363488	1
FIEBIG	Mannitol	191654012	1
Fischar/Noweda	Mannitol	18E25-B09	1
Fragon/ Gehe	Mannitol	18103b06357782	1
Fragon	Mannitol	18D09-B13-352214	1
FragonFiebig	Mannitol	18A30-B07-348872	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fragron/ Alliance	Mannitol	19C11-B04	1
Fragron/Noweda	Mannitol	17A12-B04-330729	1
Gatt-Koller	Mannitol	1803827	2
gehe 10.12.13	Mannitol	1305043/01	1
GEHE 24.07.2014	Mannitol	1310004-02	1
Gehe/ Eurho	Mannitol	1205016-02	1
Gehe/Euro	Mannitol	1511025-01	1
Gehe	Mannitol	12E24-N08	1
Gehe	Mannitol	12J26-N15	1
GEHE	Mannitol	130504301	1
Gehe	Mannitol	13E24-N01	1
Gehe	Mannitol	150202201	1
Gehe	Mannitol	1508012-01	1
Gehe	Mannitol	15197313	1
Gehe	Mannitol	1606031-01	1
Gehe	Mannitol	16200913	1
Gehe	Mannitol	17045009	1
GEHE	Mannitol	17258808	1
Gehe	Mannitol	17258812	1
Gehe	Mannitol	17360101	2
GEHE	Mannitol	17B08-B04-334312	1
Gehe	Mannitol	17F27-B05-337913	1
Gehe	Mannitol	17L04-B03-345230	1
Gehe	Mannitol	1908019-01	1
Gehe	Mannitol	19B12-B02-359604	1
Gehe	Mannitol	2008030-01	1
Gehe	Mannitol	21003432002	1
Gehe	Mannitol	2108014-01	2
Gehe	Mannitol	21K16-B11-216336	1
Gehe	Mannitol	22001495041	1
Gehe	Mannitol	22001712012	1
Gehe	Mannitol	2209020-01	1
Gehe	Mannitol	23A10-F13-384085	1
Gutenberg-Apotheke	Mannitol	1310004-01	4
Gutenberg-Apotheke	Mannitol	1310004-02	1
Gutenberg-Apotheke	Mannitol	13189221	1
Hirsch	Mannitol	12305725	1
INTERN-DROGEN	Mannitol	17258812	1
JENNE	Mannitol	17258811	1
Jenne	Mannitol	24000356001	3
Kehr 15.09.2020	Mannitol	20B05-F03-369844	1
Kehr	Mannitol	22F15-F18	1
Kehr	Mannitol	2307004-01	2
Klenk	Mannitol	1211034-02	2
Klenk	Mannitol	1606031-01	2
Klenk	Mannitol	17360108	1
Klenk	Mannitol	5224A110314	1
Kögl	Mannitol	1900820	1
Krieger	Mannitol	20F12-F10-373771	1
Krieger	Mannitol	20L15-F15-376869	1
Linden-Apotheke	Mannitol	1205016-02	1
Noewda	Mannitol	15197319	1
Noweda Frechen	Mannitol	20J06F13375106	1
Noweda/Fragron	Mannitol	18E25-B07-352753	1
Noweda/Fragron	Mannitol	19D16-B04	1
Noweda	Mannitol	11219101	2
Noweda	Mannitol	11219138	1
Noweda	Mannitol	1205016-02	2
Noweda	Mannitol	12105404	1
Noweda	Mannitol	1305043-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Mannitol	14323124	1
Noweda	Mannitol	1508012-01	1
Noweda	Mannitol	1511025-01	1
Noweda	Mannitol	15B05-B06-304302	1
Noweda	Mannitol	15I24-B05-314323	1
Noweda	Mannitol	15K17-B01	1
Noweda	Mannitol	15l24-B05-314323	1
Noweda	Mannitol	16D20-B04-320487	1
Noweda	Mannitol	16L15-B05-329316	1
Noweda	Mannitol	17045002	1
Noweda	Mannitol	1708005-01	3
Noweda	Mannitol	17258812	1
Noweda	Mannitol	1809008-02	1
Noweda	Mannitol	18B23-B10	1
Noweda	Mannitol	18L03-B06-357782	1
Noweda	Mannitol	1904025-01	1
Noweda	Mannitol	19D16-B03	1
Noweda	Mannitol	20004038003	1
Noweda	Mannitol	21K16-B11-216336	1
Noweda	Mannitol	22001712011	1
Noweda	Mannitol	2201036-01	1
Noweda	Mannitol	23A10-F03	1
Noweda	Mannitol	P101P102P103	3
Noweda29.04.2015	Mannitol	14323113	1
Phagron	Mannitol	1302C004-279405	1
PHOENIX 24.04.2014	Mannitol	1310004-01	3
Phoenix WE 10.03.17 ...	Mannitol	16340302	1
Phoenix/Fragon	Mannitol	17B08-B04-334314	1
Phoenix	Mannitol	120501602	1
Phoenix	Mannitol	1310004-01	1
Phoenix	Mannitol	15197314	1
Phoenix	Mannitol	15197319	1
Phoenix	Mannitol	1708005-01	2
Phoenix	Mannitol	18265503	1
Phoenix	Mannitol	18265506	1
Phoenix	Mannitol	18L21-B04-358870	1
Phoenix	Mannitol	19B12-B03	1
Phoenix	Mannitol	19C11-B03-361202	1
Phoenix	Mannitol	20000958001	1
Phoenix	Mannitol	20003605013	1
Phoenix	Mannitol	200180502	1
Phoenix	Mannitol	200331404	1
Phönix WE:02.08.201...	Mannitol	15197313	1
Phönix Gotha	Mannitol	19I20-F09	1
Phönix/ Caesar&Loret...	Mannitol	20000958003	1
Phönix	Mannitol	120501602	1
Phönix	Mannitol	1211034-02	1
Phönix	Mannitol	12305723	1
Phönix	Mannitol	1305043-01	1
Phönix	Mannitol	14051215	1
phönix	Mannitol	14323138	1
phönix	Mannitol	15197313	2
PHÖNIX	Mannitol	16200923	1
Phönix	Mannitol	16200924	2
PHÖNIX	Mannitol	16212102	1
Phönix	Mannitol	17045008	1
Phönix	Mannitol	17258819	1
PHÖNIX	Mannitol	17258821	1
PHÖNIX	Mannitol	17258823	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Mannitol	17360109	1
Phönix	Mannitol	18265411	1
Phönix	Mannitol	18265429	1
Phönix	Mannitol	18L21-B04	1
Phönix	Mannitol	20H21-F06-373986	1
Phönix	Mannitol	22822-F08	1
PHÖNIX	Mannitol	22A12F04-381467	1
Phönix	Mannitol	23A10-F14-384085	1
Primavera/Phoenix	Mannitol	1708005-01	1
Retest	Mannitol	1409016-01	1
Roquette / Gehe	Mannitol	E851E	1
Roquette Lestrem/Noweda	Mannitol	1508012-01	1
Roquette Lestrem/Noweda	Mannitol	1511025-01	1
Roquette/Noweda	Mannitol	E235L	1
Roquette/Phoenix	Mannitol	E118T	1
Sana	Mannitol	17258809	2
Sanac	Mannitol	1610027-01	1
Sanacorp E.K:19,49 ...	Mannitol	17045009	1
Sanacorp 06.05.22 18,91EUR	Mannitol	22B01-F04-381542	1
Sanacorp	Mannitol	10974140	1
Sanacorp	Mannitol	1310004-01	1
Sanacorp	Mannitol	13189215	1
Sanacorp	Mannitol	14051205	1
Sanacorp	Mannitol	16200903	1
Sanacorp	Mannitol	16200924	1
Sanacorp	Mannitol	17087916	1
Sanacorp	Mannitol	17258808	1
Sanacorp	Mannitol	17258809	1
Sanacorp	Mannitol	17K29-B05	1
Sanacorp	Mannitol	1806024-01	1
Sanacorp	Mannitol	18265509	1
Sanacorp	Mannitol	1904025-02	1
Sanacorp	Mannitol	22001712004	1
Sanacorp	Mannitol	22001712011	2
Sanacorp	Mannitol	2201712011	1
Sanacorp	Mannitol	22E23-F18-382115	1
Sanacorp	Mannitol	2301038-01	1
Sanacorp	Mannitol	23A24-F03-384303	1
Sanacorp	Mannitol	24000356003	1
Sanacorp	Mannitol	24000356005	1
Sancorp/Euro OCT	Mannitol	190425-02	1
Shijiazhuang/Phoenix	Mannitol	1901092	2
Sonnen-Apotheke Wefe...	Mannitol		2
Sonnen-Apotheke Wefe...	Mannitol	4/2021	1
stumpf	Mannitol	1104028-02	1
VDL;21.11.14;3,98EUR	Mannitol	13189227	1
vwr chemicals	Mannitol	20K134121	1
vwr chemicals	Mannitol	21G264113	1
WE:16.03.2016 Sanacorp	Mannitol	14323124	1
WE:30.03.2016 Sanacorp	Mannitol	14323138	1
WE:Sanacorp 02.09.16...	Mannitol	16212101	1
WE:Sanacorp 25.10.20...	Mannitol	16212102	2
xxxxx	Mannitol	xxxx	1

- 232 796 spectra from 1515 *Apo-Ident* customers from a total of 48 394 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Mannitol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mannitol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	1670	0	200 334
Type C	0	3267	4	232 773

The substance/substance group *Mannitol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.6407 %)
Type C	100.0000 % (> 99.9005 %)	99.8777 % (> 99.7860 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20980	20980	0.00	176.70
21884	21884	0.00	177.19
22286	22286	0.00	177.46
22581	22286	2.81	180.01
22883	22286	4.40	178.69
22884	22286	4.98	178.25
24579	21884	7.81	187.39
25548	25548	0.00	178.84
26396	22286	12.81	193.04

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Melatonin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20553-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Melatonin; Melatoninum

Special notes

When selecting the *Melatonin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Melatonin	11	13	332

Second-stage model

For differentiation of the substance/substance group *Melatonin* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Melatonin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	84.77	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Melatonin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Melatonin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Melatonin	12321404	20834	40	20121107
Caelo	Melatonin	12321411	20835	40	20121107
Caelo	Melatonin	12321415	20987	80	20121107
Caelo	Melatonin	21002239029	26415	40	20210723
Caelo	Melatonin	21002239029	26415SI	40	20210723
Euro OTC	Melatonin	1305029-02	21618	60	1411054
Euro OTC	Melatonin	1510041	22237	60	20151123*
Euro OTC	Melatonin	1709020	23889	40	20180105*
Euro OTC	Melatonin	1804015	24128	40	20180522*
Euro OTC	Melatonin	1804015	24128SI	40	20180522*
Euro OTC	Melatonin	2101018	25542	40	20210202*
Euro OTC	Melatonin	2101018	25542SI	40	20210202*
Fagron	Melatonin	15G06-B03-315183	22892	40	20150717
Fagron	Melatonin	15G06-B03-323733	22893	40	20150717

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 640 spectra of 14 reference samples from the substance/substance group *Melatonin*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 322 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1019 spectra of 25 reference samples from the substance/substance group *Melatonin*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Melatonin	163437	23036	40
Caelo	Melatonin	190946	24519	40
Caelo	Melatonin	22003650	26487	40
Euro OTC	Melatonin	1610040	22871	40
Euro OTC	Melatonin	1811004	24330	40
Euro OTC	Melatonin	1906031	24767	40
Euro OTC	Melatonin	1906030	24802	40
Euro OTC	Melatonin	1909031	24924	40
Euro OTC	Melatonin	2002029	25148	40
Euro OTC	Melatonin	2106005	25766	50
Euro OTC	Melatonin	2110002	25890	50
Euro OTC	Melatonin	2309003	27283	40
Fagron	Melatonin	22I16-B05-224268	26458	40
Caelo	Melatonin	163437	23036SI	40
Caelo	Melatonin	190946	24519SI	40
Caelo	Melatonin	22003650	26487SI	40
Euro OTC	Melatonin	1510041	22237SI†	60
Euro OTC	Melatonin	1811004	24330SI	39
Euro OTC	Melatonin	2002029	25148SI	40
Euro OTC	Melatonin	2106005	25766SI	50
Euro OTC	Melatonin	2110002	25890SI	10
Euro OTC	Melatonin	2309003	27283SI	40
Fagron	Melatonin	15G06-B03-315183	22892SI†	40
Fagron	Melatonin	15G06-B03-323733	22893SI†	40
Fagron	Melatonin	22I16-B05-224268	26458SI	40

- 201 065 spectra from a total of 4029 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1695 spectra from 478 *Apo-Ident* customers from 342 batches from the substance/substance group *Melatonin*.
- Among them are spectra of independent samples from 332 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Melatonin	192978006	2
	Melatonin	20220508	1
	Melatonin	20A31-F02-372824	1
	Melatonin	20A31-F02-377484	2
	Melatonin	21002239013	1
	Melatonin	21002239023	1
	Melatonin	21002239028	2
	Melatonin	21002239030	4
	Melatonin	21002239034	1
	Melatonin	21002239035	1
	Melatonin	21002239038	11
	Melatonin	21002239039	3
	Melatonin	21002239041	1
	Melatonin	2110002-01	5
	Melatonin	22003650002	11
	Melatonin	22003650004	2
	Melatonin	22003650005	3
	Melatonin	22003650009	1
	Melatonin	22003650011	2
	Melatonin	22003650014	1
	Melatonin	2203650003	1
	Melatonin	22116-B05-228535	1
	Melatonin	22I16-B05-228535	1
	Melatonin	22I16-B05-228536	1
	Melatonin	22I16-B05-235144	1
	Melatonin	2309003-01	1
	Melatonin	B05-2285306	1
AEP	Melatonin	20001543005	1
AHD	Melatonin	21002239018	1
AHD	Melatonin	21002239038	3
AHD	Melatonin	22003650005	1
Alcon Biosciences Pr...	Melatonin	APALC/MLT/170301M	1
Alliance	Melatonin	15254307	3
Alliance	Melatonin	15254316	1
Alliance	Melatonin	21002239025	1
allianz	Melatonin	15254324	1
Alte Apotheke	Melatonin	15254328	1
Anzag	Melatonin	12321415	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
apo ident	Melatonin	1610040-02	1
Audor Pharma	Melatonin	ALC/MLT/170901	1
Audor Pharma	Melatonin	APALC/MLT/150501M	2
Audor Pharma	Melatonin	APALC/MLT/170901M	2
Audor Pharma	Melatonin	APALC/MLT/17090M	1
Bionorica Ethics	Melatonin	APALC/MLT/170901M	1
Bombastus	Melatonin	18210304	1
Caelo	Melatonin		1
Caelo	Melatonin	1(20001543007)	1
Caelo	Melatonin	10071303	1
Caelo	Melatonin	1126109	1
Caelo	Melatonin	11267102	1
Caelo	Melatonin	11267109	1
Caelo	Melatonin	11267110	1
Caelo	Melatonin	11267111	1
Caelo	Melatonin	11267119	1
Caelo	Melatonin	11267120	4
Caelo	Melatonin	11267121	1
Caelo	Melatonin	11267122	1
Caelo	Melatonin	11267126	2
Caelo	Melatonin	117305118	1
Caelo	Melatonin	120009	1
Caelo	Melatonin	12321404	3
Caelo	Melatonin	12321406	1
Caelo	Melatonin	12321411	1
Caelo	Melatonin	12321415	3
Caelo	Melatonin	12321416	5
Caelo	Melatonin	12321421	2
Caelo	Melatonin	12321422	4
Caelo	Melatonin	13167301	8
Caelo	Melatonin	13167302	1
Caelo	Melatonin	13167309	1
Caelo	Melatonin	13167310	1
Caelo	Melatonin	13167312	3
Caelo	Melatonin	13167314	5
Caelo	Melatonin	14110302	2
Caelo	Melatonin	14110305	2
Caelo	Melatonin	14110308	3
Caelo	Melatonin	14110314	2
Caelo	Melatonin	14110316	1
Caelo	Melatonin	150601	1
Caelo	Melatonin	15093001	7
Caelo	Melatonin	15093002	2
Caelo	Melatonin	15093004	2
Caelo	Melatonin	15093008	8
Caelo	Melatonin	15093010	5
Caelo	Melatonin	15093012	2
Caelo	Melatonin	15093013	2
Caelo	Melatonin	1514E-03554	1
Caelo	Melatonin	1524309	1
Caelo	Melatonin	15254305	7
Caelo	Melatonin	15254306	8
Caelo	Melatonin	15254307	14
Caelo	Melatonin	15254308	7
Caelo	Melatonin	15254313	2
Caelo	Melatonin	15254319	10
Caelo	Melatonin	15254320	4
Caelo	Melatonin	15254321	8
Caelo	Melatonin	15254324	4
Caelo	Melatonin	15254325	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Melatonin	15254327	1
Caelo	Melatonin	15254328	2
Caelo	Melatonin	15254331	8
Caelo	Melatonin	15254332	2
Caelo	Melatonin	15254333	1
Caelo	Melatonin	15254336	4
Caelo	Melatonin	15254338	6
Caelo	Melatonin	15C20B01306077	1
Caelo	Melatonin	15G06-B03-321298	2
Caelo	Melatonin	15G06-B03-321299	1
Caelo	Melatonin	15G06-B03-323733	1
Caelo	Melatonin	160125M	1
Caelo	Melatonin	16121303	1
Caelo	Melatonin	16266901	9
Caelo	Melatonin	16266903	2
Caelo	Melatonin	16266904	3
Caelo	Melatonin	16266906	4
Caelo	Melatonin	16266908	7
Caelo	Melatonin	16266909	10
Caelo	Melatonin	16266912	2
Caelo	Melatonin	163437/13	1
Caelo	Melatonin	16343702	3
Caelo	Melatonin	16343705	2
Caelo	Melatonin	16343706	2
Caelo	Melatonin	16343707	2
Caelo	Melatonin	16343708	13
Caelo	Melatonin	16343709	13
Caelo	Melatonin	16343710	12
Caelo	Melatonin	16343711	4
Caelo	Melatonin	16343712	1
Caelo	Melatonin	16343713	12
Caelo	Melatonin	17/28-B04-345376	2
Caelo	Melatonin	17/28-b04-351312	1
Caelo	Melatonin	1709020-01	2
Caelo	Melatonin	17305101	5
Caelo	Melatonin	17305101-20180206Ma1	1
Caelo	Melatonin	17305102	30
Caelo	Melatonin	17305104	4
Caelo	Melatonin	17305105	15
Caelo	Melatonin	17305106	13
Caelo	Melatonin	17305109	1
Caelo	Melatonin	17305110	7
Caelo	Melatonin	17305113	7
Caelo	Melatonin	17305114	8
Caelo	Melatonin	17305115	5
Caelo	Melatonin	17305116	4
Caelo	Melatonin	17305118	13
Caelo	Melatonin	17305119	6
Caelo	Melatonin	17305120	1
Caelo	Melatonin	17305121	5
Caelo	Melatonin	17305122	14
Caelo	Melatonin	17350119	1
Caelo	Melatonin	17C22-B01-337090	1
Caelo	Melatonin	17I28-B04-344439	2
Caelo	Melatonin	17I28-B04-345376	1
Caelo	Melatonin	17l28-B04-351312	1
Caelo	Melatonin	1810308	1
Caelo	Melatonin	182010312	1
Caelo	Melatonin	18210301	18
Caelo	Melatonin	18210303	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Melatonin	18210304	19
Caelo	Melatonin	18210306	11
Caelo	Melatonin	18210307	4
Caelo	Melatonin	18210308	5
Caelo	Melatonin	18210311	14
Caelo	Melatonin	18210312	10
Caelo	Melatonin	18210313	8
Caelo	Melatonin	18210315	1
Caelo	Melatonin	18210318	11
Caelo	Melatonin	18210319	4
Caelo	Melatonin	191280001	17
Caelo	Melatonin	191280002	12
Caelo	Melatonin	191280003	1
Caelo	Melatonin	191280005	17
Caelo	Melatonin	191280006	2
Caelo	Melatonin	191280009	16
Caelo	Melatonin	19128001	1
Caelo	Melatonin	19128003	10
Caelo	Melatonin	19128005	18
Caelo	Melatonin	19128006	20
Caelo	Melatonin	19128007	11
Caelo	Melatonin	192978004	1
Caelo	Melatonin	192978005	16
Caelo	Melatonin	192978006	17
Caelo	Melatonin	2(20001543007)	1
Caelo	Melatonin	20001543005	8
Caelo	Melatonin	20001543007	12
Caelo	Melatonin	20001543009	1
Caelo	Melatonin	20001543010	10
Caelo	Melatonin	20001543012	11
Caelo	Melatonin	20001543014	16
Caelo	Melatonin	20021312	1
Caelo	Melatonin	20021505	1
Caelo	Melatonin	2002239003	1
Caelo	Melatonin	20A31-F02-372823	1
Caelo	Melatonin	21000597001	10
Caelo	Melatonin	21000597002	1
Caelo	Melatonin	21000597003	1
Caelo	Melatonin	21002239001	1
Caelo	Melatonin	21002239003	20
Caelo	Melatonin	21002239004	2
Caelo	Melatonin	21002239005	15
Caelo	Melatonin	21002239006	8
Caelo	Melatonin	21002239008	1
Caelo	Melatonin	21002239011	8
Caelo	Melatonin	21002239013	19
Caelo	Melatonin	21002239018	3
Caelo	Melatonin	21002239021	17
Caelo	Melatonin	21002239023	10
Caelo	Melatonin	21002239028	5
Caelo	Melatonin	21002239029	7
Caelo	Melatonin	21002239030	2
Caelo	Melatonin	21002239034	9
Caelo	Melatonin	21002239035	5
Caelo	Melatonin	21002239036	3
Caelo	Melatonin	21002239039	1
Caelo	Melatonin	2100223909	1
Caelo	Melatonin	2100597002	1
Caelo	Melatonin	211002239028	1
Caelo	Melatonin	22003650002	6

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Melatonin	22003650005	1
Caelo	Melatonin	2313M03554	1
Caelo	Melatonin	2548268	1
Caelo	Melatonin	26051805	1
Caelo	Melatonin	ALC/MLT/170901	1
Caesa / Alliance Hea…	Melatonin	18210306	1
Caesar & Lorenz GmbH	Melatonin	17305106	1
Caesar & Loretz GmbH…	Melatonin	21002239013	1
Caesar & Loretz GmbH…	Melatonin	21002239035	1
Caesar & Loretz GmbH…	Melatonin	17305102	2
Caesar & Loretz GmbH…	Melatonin	17305106	1
Caesar & Loretz GmbH…	Melatonin	18210306	1
Caesar & Loretz GmbH…	Melatonin	21002239029	1
Caesar & Loretz GmbH…	Melatonin	20001543012	2
Caesar & Loretz GmbH…	Melatonin	20001543014	1
Caesar & Loretz GmbH/AHD	Melatonin	20001543010	1
Caesar & Loretz GmbH/AHD	Melatonin	21002239013	1
Caesar & Loretz GmbH…	Melatonin	192978006	4
Caesar & Loretz GmbH…	Melatonin	20001543007	2
Caesar & Loretz GmbH…	Melatonin	20001543009	1
Caesar & Loretz GmbH/Gehe	Melatonin	192978006	3
Caesar & Loretz GmbH/Gehe	Melatonin	20001543007	2
Caesar & Loretz GmbH/Gehe	Melatonin	20001543009	1
Caesar & Loretz GmbH/Gehe	Melatonin	20001543012	1
Caesar & Loretz GmbH/Gehe	Melatonin	21002239003	1
Caesar & Loretz GmbH/Gehe	Melatonin	21002239020	1
Caesar & Loretz GmbH/Gehe	Melatonin	21002239039	2
Caesar & Loretz GmbH/Gehe	Melatonin	22003650002	1
Caesar & Loretz GmbH…	Melatonin	192978004	1
Caesar & Loretz GmbH…	Melatonin	21000597002	1
Caesar & Loretz GmbH…	Melatonin	21002239021	2
Caesar & Loretz GmbH…	Melatonin	21002239030	1
Caesar & Loretz GmbH…	Melatonin	192978006	1
Caesar & Loretz GmbH…	Melatonin	21002239005	2
Caesar & Loretz GmbH…	Melatonin	191280005	1
Caesar & Loretz GmbH…	Melatonin	21002239011	1
Caesar & Loretz GmbH…	Melatonin	20001543010	1
Caesar & Loretz GmbH…	Melatonin	21002239008	1
Caesar & Loretz GmbH…	Melatonin	21002239013	1
Caesar & Loretz GmbH	Melatonin	1524517305113	1
Caesar & Loretz GmbH	Melatonin	17305105	1
Caesar & Loretz GmbH	Melatonin	17305106	1
Caesar & Loretz GmbH	Melatonin	17305118	1
Caesar & Loretz GmbH	Melatonin	18210301	2
Caesar & Loretz GmbH	Melatonin	18210304	1
Caesar & Loretz GmbH	Melatonin	18210305	2
Caesar & Loretz GmbH	Melatonin	18210306	1
Caesar & Loretz GmbH	Melatonin	18210307	1
Caesar & Loretz GmbH	Melatonin	18210311	2
Caesar & Loretz GmbH	Melatonin	18210312	2
Caesar & Loretz GmbH	Melatonin	18210313	1
Caesar & Loretz GmbH	Melatonin	18210318	2
Caesar & Loretz GmbH	Melatonin	18210319	1
Caesar & Loretz GmbH	Melatonin	18210320	1
Caesar & Loretz GmbH	Melatonin	191280001	6
Caesar & Loretz GmbH	Melatonin	191280002	4
Caesar & Loretz GmbH	Melatonin	191280003	1
Caesar & Loretz GmbH	Melatonin	191280005	7
Caesar & Loretz GmbH	Melatonin	191280006	3
Caesar & Loretz GmbH	Melatonin	191280008	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Melatonin	191280009	7
Caesar & Loretz GmbH	Melatonin	19128003	1
Caesar & Loretz GmbH	Melatonin	19128005	5
Caesar & Loretz GmbH	Melatonin	19128007	2
Caesar & Loretz GmbH	Melatonin	192978004	4
Caesar & Loretz GmbH	Melatonin	192978005	5
Caesar & Loretz GmbH	Melatonin	192978006	16
Caesar & Loretz GmbH	Melatonin	20001543005	3
Caesar & Loretz GmbH	Melatonin	20001543007	1
Caesar & Loretz GmbH	Melatonin	20001543009	1
Caesar & Loretz GmbH	Melatonin	20001543010	3
Caesar & Loretz GmbH	Melatonin	20001543012	5
Caesar & Loretz GmbH	Melatonin	20001543014	11
Caesar & Loretz GmbH	Melatonin	2002029-01	2
Caesar & Loretz GmbH	Melatonin	21000597001	5
Caesar & Loretz GmbH	Melatonin	21000597002	2
Caesar & Loretz GmbH	Melatonin	21002239003	3
Caesar & Loretz GmbH	Melatonin	21002239004	3
Caesar & Loretz GmbH	Melatonin	21002239005	11
Caesar & Loretz GmbH	Melatonin	21002239006	4
Caesar & Loretz GmbH	Melatonin	21002239008	1
Caesar & Loretz GmbH	Melatonin	21002239013	9
Caesar & Loretz GmbH	Melatonin	21002239018	2
Caesar & Loretz GmbH	Melatonin	21002239020	2
Caesar & Loretz GmbH	Melatonin	21002239021	7
Caesar & Loretz GmbH	Melatonin	21002239023	6
Caesar & Loretz GmbH	Melatonin	21002239028	2
Caesar & Loretz GmbH	Melatonin	21002239029	9
Caesar & Loretz GmbH	Melatonin	21002239030	3
Caesar & Loretz GmbH	Melatonin	21002239031	1
Caesar & Loretz GmbH	Melatonin	21002239034	2
Caesar & Loretz GmbH	Melatonin	21002239035	1
Caesar & Loretz GmbH	Melatonin	21002239036	2
Caesar & Loretz GmbH	Melatonin	22003650001	2
Caesar & Loretz GmbH	Melatonin	22003650002	2
Caesar & Loretz Hild…	Melatonin	19128006191280009	1
Caesar & Loretz/Noweda	Melatonin	19128006	1
Caesar & Loretz/Noweda	Melatonin	20001543012	1
Caesar&Loretz GmbH	Melatonin	20001543007	1
Cealo/Gehe	Melatonin	10296624	1
Cealo	Melatonin	12321422	1
Cealo	Melatonin	20001543010	1
Cealo	Melatonin	21000597001	2
EuRho/Gehe	Melatonin	2110002-01	1
Euro OTC	Melatonin	120008	1
Euro OTC	Melatonin	12001	2
Euro OTC	Melatonin	120400302	1
Euro OTC	Melatonin	1204003-02	12
Euro OTC	Melatonin	1305029-01	8
Euro OTC	Melatonin	1407028-01	1
Euro OTC	Melatonin	1407028-02	3
Euro OTC	Melatonin	151004101	3
Euro OTC	Melatonin	1510041-01	7
Euro OTC	Melatonin	15254316	1
Euro OTC	Melatonin	161004001	1
Euro OTC	Melatonin	1610040-01	6
Euro OTC	Melatonin	1610040-02	5
Euro OTC	Melatonin	170007	1
Euro OTC	Melatonin	1709020-01	14
Euro OTC	Melatonin	170920-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Melatonin	17305106	1
Euro OTC	Melatonin	17I28-B04-360883	2
Euro OTC	Melatonin	180401501	1
Euro OTC	Melatonin	1804015-01	7
Euro OTC	Melatonin	1804015-02	1
Euro OTC	Melatonin	190603001	1
Euro OTC	Melatonin	1906030-01	13
Euro OTC	Melatonin	190903101	1
Euro OTC	Melatonin	1909031-01	2
Euro OTC	Melatonin	200202901	1
Euro OTC	Melatonin	2002029-01	26
Euro OTC	Melatonin	2101018	1
Euro OTC	Melatonin	2101018-01	7
Euro OTC	Melatonin	2106005	1
Euro OTC	Melatonin	2106005-01	5
Euro OTC	Melatonin	2110002-01	14
Euro OTC	Melatonin	71296	1
Fagron	Melatonin	11/26-N07	1
Fagron	Melatonin	11F09-N02	1
Fagron	Melatonin	120009	2
Fagron	Melatonin	12G19-N03	1
Fagron	Melatonin	12I28-B04-361873	1
Fagron	Melatonin	12K13-N02	1
Fagron	Melatonin	1305029-01	1
Fagron	Melatonin	13D12N10	1
Fagron	Melatonin	13D12-N10	2
Fagron	Melatonin	13e22-n12	1
Fagron	Melatonin	13E22N12	1
Fagron	Melatonin	13E22-N12	1
Fagron	Melatonin	13H21-N06	4
Fagron	Melatonin	13H21-N065x	1
Fagron	Melatonin	13H29-B03	1
Fagron	Melatonin	13H29-B03-291180	2
Fagron	Melatonin	14G18-B01-297242	1
Fagron	Melatonin	14G18-B01-297244	1
Fagron	Melatonin	14G18-B01-297245	1
Fagron	Melatonin	150002	1
Fagron	Melatonin	15C20-B01-306077	1
Fagron	Melatonin	15C20-B01-306078	3
Fagron	Melatonin	15C20-B01-308426	3
Fagron	Melatonin	15C20-B01-308427	5
Fagron	Melatonin	15C20-B01-308428	1
Fagron	Melatonin	15C20-B01-327131	1
Fagron	Melatonin	15G06-B03-315183	5
Fagron	Melatonin	15G06-B03-318398	1
Fagron	Melatonin	15G06-B03-321298	3
Fagron	Melatonin	15G06-B03-321299	5
Fagron	Melatonin	15G06-B03-323733	2
Fagron	Melatonin	16343702	1
Fagron	Melatonin	16343708	1
Fagron	Melatonin	16G06-B01-324743	2
Fagron	Melatonin	16G06-B01-327131	4
Fagron	Melatonin	16G06-B01-329142	4
Fagron	Melatonin	17/28-B04-344438	2
Fagron	Melatonin	17/28-B04-344439	1
Fagron	Melatonin	17/28-B04-344440	3
Fagron	Melatonin	17/28-B04-347315	1
Fagron	Melatonin	17/28-B04-348747	1
Fagron	Melatonin	17/28-B04-353566	1
Fagron	Melatonin	17/28-B04-359318	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Melatonin	170007	5
Fagron	Melatonin	17128-B04-344439	1
Fagron	Melatonin	17128-B04-355634	1
Fagron	Melatonin	17128B0436869	1
Fagron	Melatonin	1728B04347313	1
Fagron	Melatonin	1728B04360882	1
Fagron	Melatonin	17C22-B01-337089	3
Fagron	Melatonin	17C22-B01-337090	4
Fagron	Melatonin	17C22-B01-337091	2
Fagron	Melatonin	17I28	2
Fagron	Melatonin	17I28-B04	2
Fagron	Melatonin	17I28-B04-344439	5
Fagron	Melatonin	17I28-B04-344440	1
Fagron	Melatonin	17I28-B04-347314	1
Fagron	Melatonin	17I28-B04-348747	3
Fagron	Melatonin	17I28-B04-351312	2
Fagron	Melatonin	17I28-B04-352328	4
Fagron	Melatonin	17I28-B04-353566	4
Fagron	Melatonin	17I28-B04-355634	2
Fagron	Melatonin	17I28-B04-355635	1
Fagron	Melatonin	17I28-B04-356971	2
Fagron	Melatonin	17I28-B04-359317	2
Fagron	Melatonin	17I28-B04-359318	1
Fagron	Melatonin	17I28-B04-360883	2
Fagron	Melatonin	17I28-B04-361869	1
Fagron	Melatonin	17I28B04361873	1
Fagron	Melatonin	17I28-B04-361873	2
Fagron	Melatonin	17l28-B04	1
Fagron	Melatonin	17l28-B04-360883	1
Fagron	Melatonin	19002851	1
Fagron	Melatonin	19003987	1
Fagron	Melatonin	1906030-01	1
Fagron	Melatonin	191280006	1
Fagron	Melatonin	19K04-F01	1
Fagron	Melatonin	19K04-F01/370622	1
Fagron	Melatonin	19K04-F01-370622	6
Fagron	Melatonin	19K04-F01-370623	2
Fagron	Melatonin	20A31-F02	5
Fagron	Melatonin	20A31-F02-372822	2
Fagron	Melatonin	20A31-F02-372823	1
Fagron	Melatonin	20A31-F02-372824	5
Fagron	Melatonin	20A31-F02-373915	2
Fagron	Melatonin	20A31-F02-377485	1
Fagron	Melatonin	21/24-Bo1-215466	1
Fagron	Melatonin	21I24-B01-215466	1
Fagron	Melatonin	21I24-B01-215649	2
Fagron	Melatonin	21I24-BO1-215649	1
Fagron	Melatonin	22A12-B09	1
Fagron	Melatonin	22A12-B09-219594	2
Fagron	Melatonin	24E09-B01-237419	1
Fagron	Melatonin	24E09-B01-240405	1
Fagron	Melatonin	B01-2156409	1
Fagron	Melatonin	F01-3706202	1
Fargon GmbH & Co.KG	Melatonin	16G06-B01-324743	1
Fargon/AHD	Melatonin	17I28-B04-356971	1
Farmalabor / Farmalabor	Melatonin	P1201556-000	1
Farmalabor	Melatonin	P1800033-000	1
Farmalabor	Melatonin	R1804925	1
Fgron	Melatonin	12G19-N03	1
GEHE 22.03.2014	Melatonin	13167302	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe amax	Melatonin	1709020-01	1
Gehe	Melatonin	11/26-N07	1
Gehe	Melatonin	11L21-N04	1
Gehe	Melatonin	12G19-N03	2
Gehe	Melatonin	13D12-N10	1
Gehe	Melatonin	13E22-N12	1
Gehe	Melatonin	1510041-01	1
Gehe	Melatonin	15254324	1
GEHE	Melatonin	17I28-B04	1
GEHE	Melatonin	17I-28-B04	1
Gehe	Melatonin	18210311	1
Gehe	Melatonin	18210320	1
Gehe	Melatonin	19128003	5
gehe	Melatonin	21002239005	1
GEHE	Melatonin	21002239028	1
Gehe	Melatonin	21002239038	1
Gehe	Melatonin	21002239039	1
gepepharm	Melatonin	15G06-B03-315183	1
Ichthyol Gesellschaft	Melatonin	16343708	1
Inresa	Melatonin	110005	1
Jacoby Gatt-Koller	Melatonin	22J00616	1
Jenne	Melatonin	22003650002	1
Kehr	Melatonin	21002239038	1
Kehr	Melatonin	21002239039	3
Koisser	Melatonin	140202	2
KS Pharma	Melatonin	XPS130428	1
Noweda	Melatonin	18210304	1
Noweda	Melatonin	18210318	1
Noweda	Melatonin	21002239006	1
Otto Geilenkirchen Aachen	Melatonin	21002239013	2
Phoenix 03.04.2014	Melatonin	12J19-N02	1
PHOENIX 14.04.2014	Melatonin	13E22-N12	1
Phoenix/Caesar & Lor…	Melatonin	21002239028	1
Phoenix	Melatonin	15C20-B01	1
Phoenix	Melatonin	16266903	1
Phoenix	Melatonin	18210315	1
Phoenix	Melatonin	191421112	1
Phoenix	Melatonin	200480406	1
Phoenix	Melatonin	200811308	1
Phoenix	Melatonin	21002239038	1
Phoenix	Melatonin	3368	1
Phönix 02.01.15	Melatonin	13H21-N06	1
Phönix 02.01.2014	Melatonin	1204003-02	1
Phönix 19.02.2014	Melatonin	13167301	2
Phönix Gotha	Melatonin	19128005	1
Phönix	Melatonin	11267111	1
phönix	Melatonin	15254308	1
Phönix	Melatonin	17305115	1
Phönix	Melatonin	18210303	2
Phönix	Melatonin	APALC/MCT17030111	1
Sanacorp Verbund	Melatonin	20A31-F02-372823	1
Sanacorp WE: 17.0518…	Melatonin	1709020-01	1
Sanacorp	Melatonin		1
Sanacorp	Melatonin	11267119	1
sanacorp	Melatonin	14110320	1
Sanacorp	Melatonin	161004001	1
Sanacorp	Melatonin	161004002	1
Sanacorp	Melatonin	17I28-B04	3
Sanacorp	Melatonin	17I28-B04-360883	1
Sanacorp	Melatonin	18210318	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Melatonin	20001543007	1
Sanacorp	Melatonin	20001543012	1
Sanacorp	Melatonin	21002239036	1
Sanacorp	Melatonin	22003650005	1
Sanacorp	Melatonin	APALC/MLT/161101M	1
Sanacorp	Melatonin	APALC/MLT/170301M	2
Sanacorp	Melatonin	APALC/MLT/170901M	1
Sanacorp	Melatonin	APMLT170901M	1
Sanacorp	Melatonin	MLT/SEP/170901	1
Sanaorp	Melatonin	16343707	1
SWATI/Phoenix	Melatonin	2002029-01	1
WE Sanacorp 28.11..2...	Melatonin	15254324	1

- 234 372 spectra from 1515 *Apo-Ident* customers from a total of 48 917 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Melatonin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Melatonin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	640	0	152 322
Type B	0	1019	0	201 065
Type C	0	1666	29	234 372

The substance/substance group *Melatonin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0625 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4112 %)
Type C	100.0000 % (> 99.9007 %)	98.2891 % (> 98.1121 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20834	22237	28.07	237.22
20835	21618	9.69	203.32
20987	21618	5.84	205.92
21618	21618	0.00	208.16
22237	22237	0.00	206.80
22892	22237	3.53	208.65
22893	22237	5.22	210.25
23889	23889	0.00	206.00
24128	24128	0.00	206.60
25542	25542	0.00	211.37
26415	24128	9.02	204.84

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Menthol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20036-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Menthol; Mentholum

Special notes

When selecting the *Menthol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Menthol	11	18	422

Second-stage model

For differentiation of the substance/substance group *Menthol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Menthol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	123.02	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Menthol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Menthol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Menthol	13377404	21443	60	20131212
Caelo	Menthol	181522	24233	40	20180625*
Caelo	Menthol	2000170	25217	40	20200608*
Euro OTC	Menthol	1403022-02	21601	45	20140408
Euro OTC	Menthol	1509045	21932	60	20151008*
Euro OTC	Menthol	1603024	22657	40	20160429*
Euro OTC	Menthol	1608012	22825	40	20160902*
Euro OTC	Menthol	2103009	25591	40	20210322*
Euro OTC	Menthol	2204013	26091	40	20220517*
Euro OTC	Menthol	2204013	26091SI	20	20220517*
Fagron	Menthol	16L20-T04-044769	23596	40	20170116
Fagron	Menthol	18L04-T06-065445	24690	40	20181217

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 505 spectra of 12 reference samples from the substance/substance group *Menthol*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.
- 152 457 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 805 spectra of 21 reference samples from the substance/substance group *Menthol*.
- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Menthol	160956	22452	60
Caelo	Menthol	170927	23312	40
Caelo	Menthol	171889	23668	40
Caelo	Menthol	183286	24666	40
Caelo	Menthol	192453	24877	40
Caelo	Menthol	20003371	25617	40
Caelo	Menthol	21000696	25655	40
Caelo	Menthol	22000117	26019	40
Caelo	Menthol	23003505	27131	40
Euro OTC	Menthol	1701014	23005	40
Euro OTC	Menthol	1705022	23427	40
Euro OTC	Menthol	1802003	23951	40
Euro OTC	Menthol	1905013	24599	40
Euro OTC	Menthol	1912006	25089	40
Euro OTC	Menthol	2009021	25425	40
Euro OTC	Menthol	2301002	26515	40
Euro OTC	Menthol	2307028	26869	40
Fagron	Menthol	22L03-B08-227346	26537	40
Caelo	Menthol	170927	23645	40
Caelo	Menthol	22000117	26019SI	10
Euro OTC	Menthol	1403022-02	21601†	15

- 201 279 spectra from a total of 4026 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2431 spectra from 1049 *Apo-Ident* customers from 434 batches from the substance/substance group *Menthol*.
- Among them are spectra of independent samples from 422 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Menthol	1187170	1
	Menthol	1291910	1
	Menthol	21000696016	1
	Menthol	21000696018	1
	Menthol	21000730009	1
	Menthol	21000730016	2
	Menthol	2103009-01	1
	Menthol	220003309003	1
	Menthol	22002585003	6
	Menthol	22003309002	1
	Menthol	22003309003	10
	Menthol	22003309005	2
	Menthol	22003309007	5
	Menthol	22003309012	1
	Menthol	2204013-01	4
	Menthol	2204013-02	1
	Menthol	22A14-B05-219347	4
	Menthol	22F02-B11	1
	Menthol	22F02-B11-222586	7
	Menthol	22F02-B11-22586	1
	Menthol	22F02-B11-222586	1
	Menthol	2301002-01	18
	Menthol	2301002-02	7
	Menthol	2307028-01	3
	Menthol	23B14-B26-227532	6
	Menthol	B03-2193406	1
08639701	Menthol	2301002-01	1
11,22	Menthol	21C12-B03-211790	1
AHC	Menthol	22F02-B11-222586	1
AHD	Menthol	1305010-01	1
AHD	Menthol	18128014	1
AHD	Menthol	21000696018	1
AHD	Menthol	23G19-B06-231924	1
Alliance Health 14.04..14	Menthol	1305010-02	1
Alliance Healthcare	Menthol	15363804	1
Alliance Healthcare	Menthol	19162801	1
Alliance Healthcare	Menthol	23G19-B06-231924	1
alliance	Menthol	21000730009	1
Andreas Imhof	Menthol	8052015	1
Anzag	Menthol	12/19-N10	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Anzag	Menthol	16L20-T04-044769	1
Apo-ident	Menthol	1509045-03	1
apo-ident	Menthol	1705022-01	1
apoident	Menthol	1807044-01	1
Audor Pharma	Menthol	200902102	1
beyvers	Menthol	16095613	1
Bombastus	Menthol	16095620	1
Bombastus	Menthol	16L20-T04-053177	1
Caeelo/Noweda	Menthol	20000970006	1
Caele	Menthol	2004420002	1
Caelo	Menthol		4
Caelo	Menthol	1/AD1	1
Caelo	Menthol	10008029-02	1
Caelo	Menthol	10157615	1
Caelo	Menthol	1046973	2
Caelo	Menthol	1087209	1
Caelo	Menthol	11091405	1
Caelo	Menthol	1115262	2
Caelo	Menthol	1119I-01855	1
Caelo	Menthol	11202901	1
Caelo	Menthol	11202910	5
Caelo	Menthol	12020402	5
Caelo	Menthol	1202041	1
Caelo	Menthol	12020410	1
Caelo	Menthol	12020411	8
Caelo	Menthol	1204036-01	1
Caelo	Menthol	12246203	1
Caelo	Menthol	12246204	1
Caelo	Menthol	12246205	8
Caelo	Menthol	12246211	3
Caelo	Menthol	130501001	1
Caelo	Menthol	13102001	1
Caelo	Menthol	13103802	1
Caelo	Menthol	13103901	24
Caelo	Menthol	13159104	4
Caelo	Menthol	13159105	20
Caelo	Menthol	13159110	2
Caelo	Menthol	1320260	2
Caelo	Menthol	13377402	3
Caelo	Menthol	13377404	17
Caelo	Menthol	13377407	2
Caelo	Menthol	13377408	2
Caelo	Menthol	13377409	9
Caelo	Menthol	133774112	1
Caelo	Menthol	13377412	3
Caelo	Menthol	13377413	1
Caelo	Menthol	13D1N09	1
Caelo	Menthol	13G09-N09	1
Caelo	Menthol	1403022-01	1
Caelo	Menthol	1403022-02	1
Caelo	Menthol	1410004-01	2
Caelo	Menthol	1410004-02	2
Caelo	Menthol	14183004	14
Caelo	Menthol	14183006	1
Caelo	Menthol	14183008	3
Caelo	Menthol	14183011	2
Caelo	Menthol	14183012	3
Caelo	Menthol	14183014	2
Caelo	Menthol	14183017	3
Caelo	Menthol	14183020	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Menthol	1507601	1
Caelo	Menthol	15076101	8
Caelo	Menthol	15076104	1
Caelo	Menthol	15076106	12
Caelo	Menthol	15076112	10
Caelo	Menthol	15076113	9
Caelo	Menthol	15076115	3
Caelo	Menthol	15076118	2
Caelo	Menthol	15076215	1
Caelo	Menthol	15076219	1
Caelo	Menthol	1509045-03	1
Caelo	Menthol	15286201	1
Caelo	Menthol	15286205	1
Caelo	Menthol	15286209	1
Caelo	Menthol	15286212	2
Caelo	Menthol	15286216	1
Caelo	Menthol	15363803	2
Caelo	Menthol	15363804	11
Caelo	Menthol	15363805	11
Caelo	Menthol	15363809	8
Caelo	Menthol	15363810	13
Caelo	Menthol	15363815	16
Caelo	Menthol	1536815	1
Caelo	Menthol	1603024-01	3
Caelo	Menthol	160719M	1
Caelo	Menthol	1608012-01	2
Caelo	Menthol	1608012-02	4
Caelo	Menthol	16081805	1
Caelo	Menthol	160956	1
Caelo	Menthol	16095601	1
Caelo	Menthol	16095602	3
Caelo	Menthol	16095603	5
Caelo	Menthol	16095604	1
Caelo	Menthol	16095606	17
Caelo	Menthol	16095609	1
Caelo	Menthol	16095613	13
Caelo	Menthol	16095614	16
Caelo	Menthol	16095616	1
Caelo	Menthol	16095617	2
Caelo	Menthol	16095619	17
Caelo	Menthol	16095620	9
Caelo	Menthol	160956217188904	1
Caelo	Menthol	16095625	2
Caelo	Menthol	16098614	1
Caelo	Menthol	161202M/15076111	1
Caelo	Menthol	16L20-T04-053177	1
Caelo	Menthol	1701014-01	3
Caelo	Menthol	170101402	1
Caelo	Menthol	1701014-02	2
Caelo	Menthol	170502201	1
Caelo	Menthol	1705022-01	9
Caelo	Menthol	17072001	1
Caelo	Menthol	17078004	2
Caelo	Menthol	17078006	2
Caelo	Menthol	17078009	1
Caelo	Menthol	170822M/16095616	1
Caelo	Menthol	17188903	25
Caelo	Menthol	171889035483	1
Caelo	Menthol	17188904	24
Caelo	Menthol	17188906	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Menthol	17328803	5
Caelo	Menthol	17328804	19
Caelo	Menthol	17351501	2
Caelo	Menthol	17351505	7
Caelo	Menthol	17351506	1
Caelo	Menthol	1738804	1
Caelo	Menthol	1802003-01	3
Caelo	Menthol	18128007	5
Caelo	Menthol	18128008	7
Caelo	Menthol	18128009	19
Caelo	Menthol	18128012	1
Caelo	Menthol	18128014	1
Caelo	Menthol	18128015	20
Caelo	Menthol	18128015P-190718-7	1
Caelo	Menthol	18152202	4
Caelo	Menthol	18152205	5
Caelo	Menthol	18152210	2
Caelo	Menthol	18152214	2
Caelo	Menthol	18152216	2
Caelo	Menthol	1832605	1
Caelo	Menthol	18326805	1
Caelo	Menthol	18328601	3
Caelo	Menthol	18328604	2
Caelo	Menthol	18328605	31
Caelo	Menthol	18328610	3
Caelo	Menthol	18328611	1
Caelo	Menthol	18328612	28
Caelo	Menthol	1838605	1
Caelo	Menthol	18L04-T06-065445	2
Caelo	Menthol	190501301	1
Caelo	Menthol	190513-02	1
Caelo	Menthol	19051401	1
Caelo	Menthol	19091805	1
Caelo	Menthol	19162801	6
Caelo	Menthol	19245006	1
Caelo	Menthol	1924530006	1
Caelo	Menthol	192453004	1
Caelo	Menthol	192453006	21
Caelo	Menthol	192977003	2
Caelo	Menthol	192977004	8
Caelo	Menthol	20000970006	4
Caelo	Menthol	20001704005	3
Caelo	Menthol	20004049004	5
Caelo	Menthol	20004049007	3
Caelo	Menthol	20004420002	19
Caelo	Menthol	20004420003	1
Caelo	Menthol	2000442002	3
Caelo	Menthol	20044200002	1
Caelo	Menthol	20200712-2	1
Caelo	Menthol	20E22-B02-2025100	1
Caelo	Menthol	21000696007	1
Caelo	Menthol	21000696010	6
Caelo	Menthol	210006960100	1
Caelo	Menthol	21000696012	9
Caelo	Menthol	21000696015	5
Caelo	Menthol	21000696016	2
Caelo	Menthol	21000696017	1
Caelo	Menthol	21000730002	1
Caelo	Menthol	21000730003	19
Caelo	Menthol	21000730006	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Menthol	21000730007	1
Caelo	Menthol	21000730009	6
Caelo	Menthol	21000730010	1
Caelo	Menthol	21000730011	12
Caelo	Menthol	21000730012	1
Caelo	Menthol	21000730016	6
Caelo	Menthol	2100073011	1
Caelo	Menthol	2100080011	1
Caelo	Menthol	2100096015	1
Caelo	Menthol	2100696007	1
Caelo	Menthol	211227(21000730003)	1
Caelo	Menthol	21C12-B03-211790	1
Caelo	Menthol	21C12-B03-2117900	1
Caelo	Menthol	22003309003	1
Caelo	Menthol	2204013-01	1
Caelo	Menthol	22042002	1
Caelo	Menthol	220622(21000730009)	1
Caelo	Menthol	2416	1
Caelo	Menthol	25041402	1
Caelo	Menthol	25051301	1
Caelo	Menthol	2912110 3	1
Caelo	Menthol	314Q01855	1
Caelo	Menthol	3912A-01855	1
Caelo	Menthol	4137664	1
Caelo	Menthol	5117A-01855	1
Caelo	Menthol	515M-01855	1
Caelo	Menthol	5315I-01855	1
Caelo	Menthol	617E-01855	1
Caelo	Menthol	62470307	1
Caelo	Menthol	687711	1
Caelo	Menthol	7111201	1
Caelo	Menthol	72173258	1
Caelo	Menthol	750137	1
Caelo	Menthol	814A-01855	1
Caelo	Menthol	90(17328804)	1
Caelo	Menthol	91(18128009)	1
Caelo	Menthol	92(18128015)	1
Caelo	Menthol	930716	1
Caelo	Menthol	97(192453006)	1
Caelo	Menthol	98(20004420002)	1
Caelo	Menthol	AP210305-02	1
Caelo	Menthol	IntCh311052	1
Caeolo/Gehe	Menthol	16096619	1
Caesar & Lorenz GmbH	Menthol	15076101	1
Caesar & Loretz GmbH…	Menthol	20004049007	1
Caesar & Loretz GmbH…	Menthol	21000696010	1
Caesar & Loretz GmbH…	Menthol	21000730009	2
Caesar & Loretz GmbH…	Menthol	11202910	1
Caesar & Loretz GmbH…	Menthol	12020402	1
Caesar & Loretz GmbH…	Menthol	12020411	1
Caesar & Loretz GmbH…	Menthol	13103901	1
Caesar & Loretz GmbH…	Menthol	18128009	1
Caesar & Loretz GmbH…	Menthol	18328605	1
Caesar & Loretz GmbH…	Menthol	1912006-01	3
Caesar & Loretz GmbH/A	Menthol	21003010002	1
Caesar & Loretz GmbH/AHD	Menthol	192453006	2
Caesar & Loretz GmbH/AHD	Menthol	21000730003	1
Caesar & Loretz GmbH…	Menthol	20004420002	1
Caesar & Loretz GmbH…	Menthol	18328612	2
Caesar & Loretz GmbH…	Menthol	20004420002	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Menthol	21000730011	1
Caesar & Loretz GmbH/G	Menthol	20004049007	1
Caesar & Loretz GmbH/Gehe	Menthol	18128015	1
Caesar & Loretz GmbH/Gehe	Menthol	191628	1
Caesar & Loretz GmbH/Gehe	Menthol	20004049007	1
Caesar & Loretz GmbH/Gehe	Menthol	21000696010	1
Caesar & Loretz GmbH/Gehe	Menthol	21000730016	2
Caesar & Loretz GmbH...	Menthol	18328605	1
Caesar & Loretz GmbH...	Menthol	22002585003	1
Caesar & Loretz GmbH...	Menthol	AP220321-05	1
Caesar & Loretz GmbH/Nowe	Menthol	20001704005	1
Caesar & Loretz GmbH...	Menthol	18152202	1
Caesar & Loretz GmbH...	Menthol	18328605	3
Caesar & Loretz GmbH...	Menthol	21000730003	1
Caesar & Loretz GmbH...	Menthol	192453006	1
Caesar & Loretz GmbH...	Menthol	20000970006	1
Caesar & Loretz GmbH...	Menthol	20004049004	1
Caesar & Loretz GmbH...	Menthol	192977004	1
Caesar & Loretz GmbH...	Menthol	192453006	1
Caesar & Loretz GmbH...	Menthol	20004420002	1
Caesar & Loretz GmbH...	Menthol	21000696012	1
Caesar & Loretz GmbH...	Menthol	21000730003	1
Caesar & Loretz GmbH...	Menthol	22003309003	1
Caesar & Loretz GmbH/Sana	Menthol	20000970006	1
Caesar & Loretz GmbH...	Menthol	17328804	1
Caesar & Loretz GmbH...	Menthol	192453006	1
Caesar & Loretz GmbH...	Menthol	20004049004	1
Caesar & Loretz GmbH...	Menthol	21000730006	1
Caesar & Loretz GmbH...	Menthol	21000730016	1
Caesar & Loretz GmbH...	Menthol	AP210401-02	1
Caesar & Loretz GmbH	Menthol	17328804	1
Caesar & Loretz GmbH	Menthol	18128007	2
Caesar & Loretz GmbH	Menthol	18128009	5
Caesar & Loretz GmbH	Menthol	18128015	2
Caesar & Loretz GmbH	Menthol	18152210	1
Caesar & Loretz GmbH	Menthol	183286001	3
Caesar & Loretz GmbH	Menthol	18328603	2
Caesar & Loretz GmbH	Menthol	18328604	3
Caesar & Loretz GmbH	Menthol	18328605	7
Caesar & Loretz GmbH	Menthol	18328610	1
Caesar & Loretz GmbH	Menthol	18328611	1
Caesar & Loretz GmbH	Menthol	18328612	7
Caesar & Loretz GmbH	Menthol	1905013-01	1
Caesar & Loretz GmbH	Menthol	19162801	2
Caesar & Loretz GmbH	Menthol	192453004	3
Caesar & Loretz GmbH	Menthol	192453006	11
Caesar & Loretz GmbH	Menthol	192453008	1
Caesar & Loretz GmbH	Menthol	192977004	4
Caesar & Loretz GmbH	Menthol	20000970007	1
Caesar & Loretz GmbH	Menthol	20001704005	2
Caesar & Loretz GmbH	Menthol	20004049004	1
Caesar & Loretz GmbH	Menthol	20004049007	4
Caesar & Loretz GmbH	Menthol	20004420001	1
Caesar & Loretz GmbH	Menthol	20004420002	14
Caesar & Loretz GmbH	Menthol	20004420003	1
Caesar & Loretz GmbH	Menthol	21000696010	1
Caesar & Loretz GmbH	Menthol	21000696012	1
Caesar & Loretz GmbH	Menthol	21000730002	1
Caesar & Loretz GmbH	Menthol	21000730003	8
Caesar & Loretz GmbH	Menthol	21000730009	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Menthol	21000730010	1
Caesar & Loretz GmbH	Menthol	21000730011	5
Caesar & Loretz GmbH	Menthol	21000730016	4
Caesar & Loretz GmbH	Menthol	22003309004	2
Caesar & Loretz	Menthol	15363809	1
Caesar & Loretz	Menthol	18128007	1
Caesar&Lorenz	Menthol	21000696007	1
Caesar&Loretz GmbH	Menthol	21000730003	1
Caesar&Loretz,Phönix	Menthol	15076106	1
Caesar/Noweda	Menthol	12020403	1
Caesar/Noweda	Menthol	12246211	1
Caesar/Noweda	Menthol	15076111	2
Cealo	Menthol	1705022-01	1
Celo/AHD	Menthol	16095620	1
Defektur	Menthol	18328612	1
E Plus	Menthol	1705022-01	1
Eur Rho	Menthol	1912006-01	1
EuRho/ Gehe	Menthol	1807044-01	1
EuRho/ Noweda	Menthol	2009021-01	1
EuRho/Alliance	Menthol	1701014-01	1
EuRho/Alliance	Menthol	1905013-02	1
EuRho/Fiebig	Menthol	1905013-01	1
EuRho/Fiebig	Menthol	2103009-02	1
EuRho/Gehe	Menthol	1807044-01	1
EuRho/Jenne	Menthol	180704401	1
EuRho/Jenne	Menthol	2103009-01euri	1
EuRho/Phönix	Menthol	1146105	1
Eurho/Phönix	Menthol	2009021-01	1
Eurho/Sanacorp	Menthol	1802003-01	1
EuRho/sanacorp	Menthol	1905013-01	1
EuRho	Menthol	1046973	1
EuRho	Menthol	1204036-02	1
EuRho	Menthol	1305010-01	1
EuRho	Menthol	1603024-01	1
EuRho	Menthol	1701014-02	1
Eurho	Menthol	170502201	1
EuRho	Menthol	1705022-01	2
EuRho	Menthol	1905013-01	1
EuRho	Menthol	1912006-01	1
euRho	Menthol	200902101	1
EuRho	Menthol	2103009-03	1
EuRho	Menthol	2910A-01855	1
EuRho	Menthol	915A-01855	1
Eurho-Phönix	Menthol	2204013-01	1
Euro OTC	Menthol	1001505	3
Euro OTC	Menthol	1001506	1
Euro OTC	Menthol	1002019-03	1
Euro OTC	Menthol	1008029-01	1
Euro OTC	Menthol	1046973	1
Euro OTC	Menthol	1087209	1
Euro OTC	Menthol	1105028-01	1
Euro OTC	Menthol	1111020-01	1
Euro OTC	Menthol	1146105	6
Euro OTC	Menthol	1178546	2
Euro OTC	Menthol	1201416	1
Euro OTC	Menthol	1204036-01	8
Euro OTC	Menthol	120403602	1
Euro OTC	Menthol	1204036-02	3
Euro OTC	Menthol	120-4036-02	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Menthol	1204036-1	1
Euro OTC	Menthol	1210017-01	4
Euro OTC	Menthol	1210017-02	12
Euro OTC	Menthol	1221331	5
Euro OTC	Menthol	130501001	1
Euro OTC	Menthol	1305010-01	7
Euro OTC	Menthol	130501002	1
Euro OTC	Menthol	1305010-02	6
Euro OTC	Menthol	1310J-01855	1
Euro OTC	Menthol	1337745	1
Euro OTC	Menthol	140302201	2
Euro OTC	Menthol	1403022-01	2
Euro OTC	Menthol	1403022-02	11
Euro OTC	Menthol	14030222-02	1
Euro OTC	Menthol	140322-01	1
Euro OTC	Menthol	141000401	1
Euro OTC	Menthol	1410004-01	21
Euro OTC	Menthol	1410004-02	12
Euro OTC	Menthol	14183012	1
Euro OTC	Menthol	15020006-02	1
Euro OTC	Menthol	1502006	1
Euro OTC	Menthol	150200601	1
Euro OTC	Menthol	1502006-01	18
Euro OTC	Menthol	1502006-02	17
Euro OTC	Menthol	1509045	2
Euro OTC	Menthol	1509045-01	4
Euro OTC	Menthol	150904502	1
Euro OTC	Menthol	1509045-02	11
Euro OTC	Menthol	15-0904502	1
Euro OTC	Menthol	1509045-03	15
Euro OTC	Menthol	1602024-01	1
Euro OTC	Menthol	1603021-01	1
Euro OTC	Menthol	1603024-01	46
Euro OTC	Menthol	160801201	2
Euro OTC	Menthol	1608012-01	25
Euro OTC	Menthol	1608012-02	14
Euro OTC	Menthol	1608012-1	1
Euro OTC	Menthol	1608012-12	1
Euro OTC	Menthol	16095614	1
Euro OTC	Menthol	16L20-T04-053177	1
Euro OTC	Menthol	1701014_01	1
Euro OTC	Menthol	17010140	1
Euro OTC	Menthol	170101401	1
Euro OTC	Menthol	1701014-01	20
Euro OTC	Menthol	170101402	4
Euro OTC	Menthol	1701014-02	23
Euro OTC	Menthol	1701014-2	1
Euro OTC	Menthol	170104-01	1
Euro OTC	Menthol	17050022-01	1
Euro OTC	Menthol	1705011-01	1
Euro OTC	Menthol	1705022	1
Euro OTC	Menthol	170502201	2
Euro OTC	Menthol	1705022-01	48
Euro OTC	Menthol	1705022011	1
Euro OTC	Menthol	1705022-1	1
Euro OTC	Menthol	1802003	1
Euro OTC	Menthol	1802003/01	1
Euro OTC	Menthol	180200301	4
Euro OTC	Menthol	1802003-01	59
Euro OTC	Menthol	1807044_01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Menthol	180704401	1
Euro OTC	Menthol	1807044-01	44
Euro OTC	Menthol	180704402	1
Euro OTC	Menthol	1807044-02	5
Euro OTC	Menthol	18121718	1
Euro OTC	Menthol	182003-01	1
Euro OTC	Menthol	1905013	2
Euro OTC	Menthol	1905013_01	1
Euro OTC	Menthol	190501301	1
Euro OTC	Menthol	1905013-01	29
Euro OTC	Menthol	1905013-02	17
Euro OTC	Menthol	1905013-023	1
Euro OTC	Menthol	191080810	1
Euro OTC	Menthol	1912006-01	47
Euro OTC	Menthol	1912006-1	1
Euro OTC	Menthol	195013-01	1
Euro OTC	Menthol	1987209	1
Euro OTC	Menthol	20009021	1
Euro OTC	Menthol	200902101	1
Euro OTC	Menthol	2009021-01	60
Euro OTC	Menthol	2009021-02	11
Euro OTC	Menthol	20116	1
Euro OTC	Menthol	2103009	1
Euro OTC	Menthol	210300901	5
Euro OTC	Menthol	2103009-01	41
Euro OTC	Menthol	2103009-02	11
Euro OTC	Menthol	2103009-03	14
Euro OTC	Menthol	2201013-01	1
Euro OTC	Menthol	220401301	1
Euro OTC	Menthol	2204013-01	14
Euro OTC	Menthol	2204013-02	5
Euro OTC	Menthol	2301002-01	5
Euro OTC	Menthol	25021709	1
Euro OTC	Menthol	5116U-01855	4
Euro OTC	Menthol	6102014B	1
Euro OTC	Menthol	696773	1
Euro OTC	Menthol	721123	1
Euro OTC	Menthol	807044-011	1
Euro OTC	Menthol	807862	1
Euro OTC	Menthol	858607	1
Euro OTC	Menthol	902-012	1
Euro OTC	Menthol	973192	3
Euro OTC	Menthol	B02-2025100	1
Euro OTC	Menthol	EN/20/01001	1
Euro OTC	Menthol	PM14	1
Euro Ph. / Gehe	Menthol	1701014-02	1
Euro/Jenne	Menthol	1807044-02	1
Euro/Phönix	Menthol	1905013-02	1
Euron	Menthol	1705022-01	1
Euron	Menthol	1905013-02	1
Euroo/Phönix	Menthol	210300901	1
Europharm	Menthol	130501-01	1
F/P	Menthol	20E22B022025010	1
Fagron	Menthol	1084145	1
Fagron	Menthol	1115262	4
Fagron	Menthol	11C01-N01	1
Fagron	Menthol	11G19-N07	1
Fagron	Menthol	12/19-N10	1
Fagron	Menthol	12/19-N100554/560	1
Fagron	Menthol	1201416	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Menthol	1219-N10	1
Fagron	Menthol	1247454	4
Fagron	Menthol	1289677	2
Fagron	Menthol	12C05-N03	1
Fagron	Menthol	12Cos-N03	1
Fagron	Menthol	12D23-N06	6
Fagron	Menthol	12F01-N14	3
Fagron	Menthol	12G20-N02	3
Fagron	Menthol	12I19-N10	2
Fagron	Menthol	13D16-N09	7
Fagron	Menthol	13D16-N090631/1300	1
Fagron	Menthol	13G09-N09	1
Fagron	Menthol	13G09-N090204/520	1
Fagron	Menthol	13J21-N04	2
Fagron	Menthol	13O16-N09	1
Fagron	Menthol	14100041-01	1
Fagron	Menthol	14H29-M02	11
Fagron	Menthol	14H29-M04	1
Fagron	Menthol	15076101	1
Fagron	Menthol	15076115	1
Fagron	Menthol	1509045-03	1
Fagron	Menthol	16L20-T04	4
Fagron	Menthol	16L20-T04-044469	1
Fagron	Menthol	16L20T04044769	1
Fagron	Menthol	16L20-T04-044769	22
Fagron	Menthol	16l20T04-053177	1
Fagron	Menthol	16L20T04053177	1
Fagron	Menthol	16L20-T04-053177	13
Fagron	Menthol	16L20-To4	1
Fagron	Menthol	1701014-02	1
Fagron	Menthol	17o1014-02	1
Fagron	Menthol	1804T06065445	1
Fagron	Menthol	1807044-01	1
Fagron	Menthol	180L04-T06-065445	1
Fagron	Menthol	18204-T06	1
Fagron	Menthol	18G02T30	1
Fagron	Menthol	18G02-T30	3
Fagron	Menthol	18G02-T30-062159	26
Fagron	Menthol	18L04-T0-065445	1
Fagron	Menthol	18L04T06	1
Fagron	Menthol	18L04-T06	2
Fagron	Menthol	18L04-T06-065445	33
Fagron	Menthol	18l04-to6-065445	1
Fagron	Menthol	18L20-T04	1
Fagron	Menthol	18LO4-TO6-65445	1
Fagron	Menthol	20a31-b05-196609	1
Fagron	Menthol	20A31-b05-196609	1
Fagron	Menthol	20A31-B05-196609	15
Fagron	Menthol	20E22-B02202510	1
Fagron	Menthol	20E22-B02-202510	11
Fagron	Menthol	20e22-bo2-202510	1
Fagron	Menthol	21/13-B03-219346	2
Fagron	Menthol	2113-B03	1
Fagron	Menthol	2113B03219346	1
Fagron	Menthol	2113-BO3-219346	1
Fagron	Menthol	21C12-B03	3
Fagron	Menthol	21c12-b03-211790	1
Fagron	Menthol	21c12-B03-211790	1
Fagron	Menthol	21C12-B03-211790	19
Fagron	Menthol	21c12-bo3-211790	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Menthol	21C12-B03-211790	1
Fagron	Menthol	21I13-B03	3
Fagron	Menthol	21I13-B03_219346	1
Fagron	Menthol	21I13-B03-219346	1
Fagron	Menthol	22A14-B05-219347	7
Fagron	Menthol	22F02-B11-222586	1
Fagron	Menthol	3-21934006	1
Fagron	Menthol	750137	1
Fagron	Menthol	778301	1
Fagron	Menthol	858607	1
Fagron	Menthol	976035	1
Fagron	Menthol	B02-2025100	1
Fagron	Menthol	B03-2117900	2
Fagron	Menthol	B03-2193406	5
Fargo/Gehe	Menthol	18G02-T30062159	1
Fargo/Gehe	Menthol	B03-2117900	1
Fargon/ Noweda	Menthol	13D16-N09	1
Fargon/GEHE	Menthol	18L04-T06-065445	1
Fargon	Menthol	18G02-T30-062159	1
Fargon	Menthol	18L04-T06-065445	1
Fargon	Menthol	20A31-B05-196609	1
Fargon	Menthol	B05-1966009	1
Fiebig	Menthol	16095625	1
Fiebig	Menthol	1705022-01	1
Fiebig	Menthol	17328803	1
Fiebig	Menthol	18L04-T06-065445	1
Finteler Apotheke	Menthol	16095614	1
Finze	Menthol	9221710	1
Fragon/Sanacorp	Menthol	16L20-T04-053177	1
Frey & Lau GmbH/Noweda	Menthol	1509045-03	2
Frey + Lau GmbH/AHD	Menthol	20A31-B05-196609	1
Frey + Lau GmbH	Menthol	21/13-B03-219346	1
Frey Lau GmbH	Menthol	1270077	2
Frey*Lau GmbH	Menthol	1305010-01	1
Frey*Lau GmbH	Menthol	973192	1
Frey+Lau GmbH / Noweda	Menthol	2009021-01	1
Frey+Lau GmbH Noweda	Menthol	1178546	1
Frey+Lau GmbH/Gehe	Menthol	1001505	1
Frey+Lau GmbH/Noweda	Menthol	1221331	1
Frey+Lau GmbH	Menthol	1178546	1
Frey+Lau GmbH	Menthol	1509045-02	1
Frey+Lau GmbH	Menthol	1603024-01	1
frey+Lau/jenne	Menthol	1087209	1
Frey+Lau	Menthol	926636	1
Gehe / Ensbona	Menthol	16L20-T04-044769	1
Gehe/ 27.10.12 EuRho	Menthol	11219216	1
Gehe	Menthol	12020411	1
Gehe	Menthol	13377412	1
Gehe	Menthol	13D16-N09	1
Gehe	Menthol	1502006-02	2
Gehe	Menthol	1608012-01	1
Gehe	Menthol	16095602	1
GEHE	Menthol	16L20-T04-044769	1
Gehe	Menthol	1705022-01	2
Gehe	Menthol	1802003-01	1
Gehe	Menthol	18128009	1
Gehe	Menthol	18128015	1
Gehe	Menthol	18G02-T30-062159	1
Gehe	Menthol	1905013-01	1
Gehe	Menthol	1905013-02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Menthol	21000696012	1
Gehe	Menthol	2103009-01	1
Gehe	Menthol	22003309007	1
Gehe	Menthol	22A14-B05-219347	1
Gehe	Menthol	22F02-B11-222586	1
gehe	Menthol	2301002-02	1
Gehe	Menthol	2301002-02	1
GEHE	Menthol	B03-2193406	1
Geibo/Euro 24.1.17	Menthol	1608012-01	3
GUMO	Menthol	20004420002	1
Hageda	Menthol	20A31-B05-196609	1
Hedinger/Phönix	Menthol	17328802	1
Hepart	Menthol	1608012-02	1
Ichthyol / Phoenix	Menthol	16095603	1
Imhof	Menthol	15-5401	1
Jenne	Menthol	180200301	1
Kehr	Menthol	16095613	1
Kehr	Menthol	16095620	1
Kehr	Menthol	1802003-01	1
Kehr	Menthol	2204013-01	1
Kloster Apotheke	Menthol	9999999999	1
L10	Menthol	1705022-01	1
L12	Menthol	1603024-01	1
L12	Menthol	1802003-01	1
L12	Menthol	1807044-01	1
Menthol/Phoenix	Menthol	16L20-T04-044769	1
Nachprüfung	Menthol	123456	1
Nachprüfung	Menthol	28511041	1
Norex Flavours Pvt. ...	Menthol	15286205	2
Norex Flavours Pvt. ...	Menthol	15286207	1
Noweda	Menthol	1001505	1
Noweda	Menthol	1204036-01	1
Noweda	Menthol	1410004-01	1
Noweda	Menthol	15363809	1
Noweda	Menthol	1701014-02	1
Noweda	Menthol	1705022-01	1
Noweda	Menthol	17188904	1
Noweda	Menthol	1807044	1
Noweda	Menthol	180704401	1
Noweda	Menthol	1807044-01	1
Noweda	Menthol	1807044-02	1
Noweda	Menthol	1905013-01	1
Noweda	Menthol	20004049007	1
Noweda	Menthol	2009021	1
Noweda	Menthol	21000730011	2
Noweda	Menthol	2103009-02	1
Noweda	Menthol	21C12-B03	1
Noweda	Menthol	21C12-B03-211790	1
Noweda	Menthol	22002986002	1
NOWEDA	Menthol	2204013-01	1
Noweda	Menthol	22F02-B11-222586	2
Noweda	Menthol	2301002-01	2
Noweda	Menthol	2301002-02	1
Pala	Menthol	1802003-01	1
Ph.Eur.9.0	Menthol	1912006-01	1
Phoenix 15.04.2014	Menthol	12246211	1
Phoenix/Cealo	Menthol	1509045-01/4116F-018	1
Phoenix	Menthol	1146105	1
Phoenix	Menthol	1403022-02	1
Phoenix	Menthol	16095617	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Menthol	16095619	1
Phoenix	Menthol	16095625	1
phoenix	Menthol	180704401	1
Phoenix	Menthol	1905013-01	1
Phoenix	Menthol	2204013-02	1
Phoenix	Menthol	2301002-01	1
PHOENIX	Menthol	2301002-02	1
Phoenix	Menthol	3127	1
Phoenix	Menthol	750137	1
Phoenix	Menthol	B04-2029402	1
Phönix Gotha	Menthol	1410004-01	1
Phönix Gotha	Menthol	18L04-T06-065445	1
Phönix/EuRo	Menthol	2009021-01	1
Phönix	Menthol	12246204	1
Phönix	Menthol	13159105	1
phönix	Menthol	15363805	1
Phönix	Menthol	1608012-02	1
Phonix	Menthol	1802003-01	1
Phönix	Menthol	1802003-01	2
Phönix	Menthol	1807044-01	1
Phönix	Menthol	18128015	1
Phönix	Menthol	1905013-01	1
Phönix	Menthol	1912006-01	1
Phönix	Menthol	2009021-01	1
Phönix	Menthol	2103009-01	1
PHÖNIX	Menthol	21C12-B03-211790	1
Phönix	Menthol	22F02-B11-222586	2
Retest	Menthol	1305010-02	1
Sanacomp	Menthol	22003309003	1
Sanacorp Stralsund	Menthol	21C12-B03-211790	1
Sanacorp WE:02.09.16…	Menthol	15363809	1
Sanacorp	Menthol	1204036-01	1
Sanacorp	Menthol	1210017-01	1
Sanacorp	Menthol	1305010-01	1
Sanacorp	Menthol	13103901	1
Sanacorp	Menthol	13377409	1
Sanacorp	Menthol	16095613	1
Sanacorp	Menthol	16095619	1
Sanacorp	Menthol	17188903	1
Sanacorp	Menthol	17188904	1
Sanacorp	Menthol	17328804	1
Sanacorp	Menthol	18328605	1
Sanacorp	Menthol	18328612	1
Sanacorp	Menthol	1912006-01	1
Sanacorp	Menthol	20004420002	1
Sanacorp	Menthol	21000696016	1
Sanacorp	Menthol	21000730003	1
Sanacorp	Menthol	21000730011	1
Sanacorp	Menthol	2103009-02	1
sanacorp	Menthol	22003309003	1
Sanacorp	Menthol	22003309007	2
Sanacorp	Menthol	2204013-01	1
Sanacorp	Menthol	2301002-01	1
Sanacorp	Menthol	6/AKD3	1
siehe protokoll	Menthol	1008029-02	1
Spangro_12.03.2019	Menthol	1802003-01	1
VDL; 9.23EUR; 28.09.15	Menthol	15076113	1
WE:Sanacorp 03.11.20…	Menthol	15363810	1

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 233 636 spectra from 1515 *Apo-Ident* customers from a total of 48 835 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Menthol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Menthol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	505	0	152 457
Type B	0	791	14	201 279
Type C	0	2425	6	233 636

The substance/substance group *Menthol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8119 %)
Type B	100.0000 % (> 99.9912 %)	98.2609 % (> 97.8882 %)
Type C	100.0000 % (> 99.9007 %)	99.7532 % (> 99.6298 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21443	22657	3.93	265.90
21601	21932	21.72	250.62
21932	21932	0.00	268.03
22657	22657	0.00	269.70
22825	22825	0.00	256.18
23596	22825	3.84	253.59
24233	24233	0.00	278.27
24690	22825	6.43	256.78
25217	25217	0.00	273.80
25591	25591	0.00	257.81
26091	26091	0.00	272.38

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Mepivacaine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20710-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mepivacaine hydrochloride; Mepivacaini hydrochloridum

Special notes

When selecting the *Mepivacaine hydrochloride* substance/substance group, the following information is displayed to the user:

- Advice: Currently no longer available from major pharmaceutical manufacturers. Therefore, batch maintenance is currently not possible.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Mepivacaine hydrochloride	5	1	10

Second-stage model

For differentiation of the substance/substance group *Mepivacaine hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Mepivacaine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Tretinoin	51.31	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Mepivacaine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Mepivacaine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Mepivacaine hydrochloride	12A20-N12	20710	40	1401555
Fagron	Mepivacaine hydrochloride	13L04-B07-297077	21672	60	AR-15-FG-007876-01
Fagron	Mepivacaine hydrochloride	19F25-B02-365217	24950	40	2007301
Fagron	Mepivacaine hydrochloride	20D24-F01-370950	25368	40	20200610
Fagron	Mepivacaine hydrochloride	22C04-B01-217581	26733	40	20220603
Fagron	Mepivacaine hydrochloride	22C04-B01-217581	26733SI	20	20220603

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 6 reference samples from the substance/substance group *Mepivacaine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.
- 152 722 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Mepivacaine hydrochloride*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Mepivacaine hydrochloride	15I16-B01-322906	23212	40

- 202 044 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 13 spectra from 8 *Apo-Ident* customers from 11 batches from the substance/substance group *Mepivacaine hydrochloride*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Mepivacaine hydrochloride	13G05-N02	1
Fagron	Mepivacaine hydrochloride	12E31-B40-305570	1
Fagron	Mepivacaine hydrochloride	12F20-N07	1
Fagron	Mepivacaine hydrochloride	13G05N02	1
Fagron	Mepivacaine hydrochloride	13G05-N02	1
Fagron	Mepivacaine hydrochloride	15E04-B04-330855	1
Fagron	Mepivacaine hydrochloride	15I16-B01	1
Fagron	Mepivacaine hydrochloride	15I16-B01-341738	1
Fagron	Mepivacaine hydrochloride	15I16-B01-356826	1
Fagron	Mepivacaine hydrochloride	15I16-B-325107	2
Fagron	Mepivacaine hydrochloride	19F25-B02	1
Sanacorp	Mepivacaine hydrochloride	19F25-B02-365217	1

- 236 054 spectra from 1515 *Apo-Ident* customers from a total of 49 247 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Mepivacaine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mepivacaine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	240	0	152 722
Type B	0	40	0	202 044
Type C	0	13	0	236 054

The substance/substance group *Mepivacaine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20710	20710	0.00	53.15
21672	21672	0.00	52.81
24950	24950	0.00	53.99
25368	21672	10.83	53.76
26733	24950	25.80	51.31

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Mesalazine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21772-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mesalazine; Mesalazinum

Special notes

When selecting the *Mesalazine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Mesalazine	8	4	22

Second-stage model

For differentiation of the substance/substance group *Mesalazine* the following second-stage model is used:

- Submodel 12

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Mesalazine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Midazolam hydrochloride	101.69	–
⋮	⋮	⋮
Clioquinol	>50	30.48
Nicotinic acid	>50	32.83
Miconazole nitrate	>50	43.94
Theophylline-ethylenediamine hydrate	>50	156.73

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Mesalazine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Mesalazine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Mesalazine	1206029-04	21772	60	AR-15-FG-011819-01
Euro OTC	Mesalazine	1206029-04	21887	60	20140923
Euro OTC	Mesalazine	1602005	22518	40	20160218*
Euro OTC	Mesalazine	1602005-01	22925	40	20160218
Euro OTC	Mesalazine	1911016	25082	40	20191218*
Euro OTC	Mesalazine	2009037	25569	40	20210114*
Fagron	Mesalazine	15H13-B06-317177	22356	60	20150827
Fagron	Mesalazine	16I28-B02-327679	22929	40	20161128
Fagron	Mesalazine	22K26-B12-224459	26732	40	20230504
Fagron	Mesalazine	22K26-B12-224459	26732SI	20	20230504

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 440 spectra of 10 reference samples from the substance/substance group *Mesalazine*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 522 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 5 reference samples from the substance/substance group *Mesalazine*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Mesalazine	1611019	22872	40
Euro OTC	Mesalazine	1902013	24477	40
Euro OTC	Mesalazine	2203020	26094	40
Fagron	Mesalazine	17A17-B03-336444	23934	40
Euro OTC	Mesalazine	2203020	26094SI	20

- 201 904 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 86 spectra from 14 *Apo-Ident* customers from 26 batches from the substance/substance group *Mesalazine*.

- Among them are spectra of independent samples from 21 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Mesalazine	21F15-F50-382143	1
	Mesalazine	21J12-B18-216345	2
Caelo	Mesalazine	18C30-B05-353048	1
Euro OTC	Mesalazine		1
Euro OTC	Mesalazine	1206029-04	1
Euro OTC	Mesalazine	1602005-01	3
Euro OTC	Mesalazine	1602005-02	7
Euro OTC	Mesalazine	1611019-01	5
Euro OTC	Mesalazine	1611019-03	2
Euro OTC	Mesalazine	190201301	1
Euro OTC	Mesalazine	1902013-01	10
Euro OTC	Mesalazine	190213-01	1
Euro OTC	Mesalazine	1911016-01	3
Euro OTC	Mesalazine	2009037-01	4
Euro OTC	Mesalazine	200903702	1
Euro OTC	Mesalazine	2203020-01	2
Euro OTC	Mesalazine	B02-3638804	1
Fagron	Mesalazine		1
Fagron	Mesalazine	1100007129	1
Fagron	Mesalazine	16I28-B02-327679	24
Fagron	Mesalazine	18C30-B05-353048	4
Fagron	Mesalazine	19G05-B02-363884	1
Fagron	Mesalazine	20J13-F07-0374998	1
Fagron	Mesalazine	20J13-F07-374998	2
Fagron	Mesalazine	21F15-F02-379144	1
Fagron	Mesalazine	21F15-F02-379244	4
Fagron	Mesalazine	21F15-F02-382144	1

- 235 981 spectra from 1515 *Apo-Ident* customers from a total of 49 233 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Mesalazine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mesalazine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	180	0	201 904
Type C	0	86	0	235 981

The substance/substance group *Mesalazine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 93.0233 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21772	21772	0.00	157.85
21887	21772	14.99	156.11
22356	22518	4.63	146.24
22518	22518	0.00	144.69
22925	22518	3.89	147.76
22929	22518	9.55	147.52
25082	25082	0.00	148.12
25569	25569	0.00	148.66
26732	22518	5.93	147.82

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Metamizol sodium monohydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	22634-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Metamizol sodium monohydrate; Metamizolum natricum monohydricum

Special notes

When selecting the *Metamizol sodium monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Metamizol sodium monohydrate	5	3	5

Second-stage model

For differentiation of the substance/substance group *Metamizol sodium monohydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Metamizol sodium monohydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	144.49	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Metamizol sodium monohydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Metamizol sodium monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Metamizol sodium monohydrate	161610	22634	40	20160714*
Caelo	Metamizol sodium monohydrate	15362816	22666	40	20151106
Caelo	Metamizol sodium monohydrate	161610	23313	40	20160714*
Caelo	Metamizol sodium monohydrate	20001888002	25388	40	20200819
Caelo	Metamizol sodium monohydrate	22001474	26241	40	20220718*
Caelo	Metamizol sodium monohydrate	22001474	26241SI	20	20220718*
Caelo	Metamizol sodium monohydrate	23003148	27111	40	20240110*
Caelo	Metamizol sodium monohydrate	23003148	27111SI	20	20240110*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 280 spectra of 8 reference samples from the substance/substance group *Metamizol sodium monohydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 682 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 130 spectra of 3 reference samples from the substance/substance group *Metamizol sodium monohydrate*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Metamizol sodium monohydrate	15362815	22726	40
Caelo	Metamizol sodium monohydrate	170584	23924	40
Caelo	Metamizol sodium monohydrate	21002292003	25900	50

- 201 954 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 18 spectra from 7 *Apo-Ident* customers from 6 batches from the substance/substance group *Metamizol sodium monohydrate*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Metamizol sodium monohydrate	16161007	1
Caelo	Metamizol sodium monohydrate	17058404	6
Caelo	Metamizol sodium monohydrate	18026504	3
Caelo	Metamizol sodium monohydrate	20001888002	3
Caelo	Metamizol sodium monohydrate	21000105002	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metamizol sodium monohydrate	21002292003	2
Caesar & Loretz GmbH	Metamizol sodium monohydrate	21000105002	1

- 236 049 spectra from 1515 *Apo-Ident* customers from a total of 49 252 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Metamizol sodium monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Metamizol sodium monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	130	0	201 954
Type C	0	18	0	236 049

The substance/substance group *Metamizol sodium monohydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.3846 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22634	22634	0.00	208.08
22666	27111	12.31	207.73
23313	23313	0.00	206.57
25388	23313	9.36	207.71
26241	26241	0.00	201.50
27111	27111	0.00	204.39

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Methacholine chloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20733-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Methacholine chloride; Methacholinii chloridum

Special notes

When selecting the *Methacholine chloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Methacholine chloride	9	5	30

Second-stage model

For differentiation of the substance/substance group *Methacholine chloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Methacholine chloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ornithine aspartate	118.89	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Methacholine chloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Methacholine chloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Methacholine chloride	13260303	21251	40	20130827
Caelo	Methacholine chloride	13260302	21420	60	20130827
Caelo	Methacholine chloride	13260302	21590	60	20130827
Caelo	Methacholine chloride	13260303	21592	60	20130827
Caelo	Methacholine chloride	162293	22635	40	20160815*
Caelo	Methacholine chloride	16229304	22661	40	20160815
Caelo	Methacholine chloride	16229301	22662	40	20160815
Euro OTC	Methacholine chloride	2001028	25249	40	20200720*
Fagron	Methacholine chloride	12F01-N04	20733	60	1403251
Fagron	Methacholine chloride	16L20-B01-329966	22976	40	20170123
Fagron	Methacholine chloride	16L20-B01-329968	22977	40	20170123

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 520 spectra of 11 reference samples from the substance/substance group *Methacholine chloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 442 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 270 spectra of 8 reference samples from the substance/substance group *Methacholine chloride*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Methacholine chloride	163299	23049	40
Caelo	Methacholine chloride	20003216002	26304	30
Caelo	Methacholine chloride	23000519	26726	40
Fagron	Methacholine chloride	17H03-B02-346564	24287	40
Fagron	Methacholine chloride	22B07-B22-23069	26823	40
Caelo	Methacholine chloride	163299	23624	40
Caelo	Methacholine chloride	20003216002	26304SI	20
Caelo	Methacholine chloride	23000519	26726SI	20

- 201 814 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 46 spectra from 23 *Apo-Ident* customers from 32 batches from the substance/substance group *Methacholine chloride*.

- Among them are spectra of independent samples from 30 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
anzag 18.12.14 25,19	Methacholine chloride	14G30-B03-296209	1
Caelo	Methacholine chloride	17D13-B04-334377	1
Caelo	Methacholine chloride	23000519001	1
Caesar & Loretz GmbH...	Methacholine chloride	23000519003	1
Euro OTC	Methacholine chloride	2001028-01	1
Fagron	Methacholine chloride	10031504	1
Fagron	Methacholine chloride	13/13-N03	2
Fagron	Methacholine chloride	13121712	1
Fagron	Methacholine chloride	13G10-N05	1
Fagron	Methacholine chloride	14G30-B03-296210	1
Fagron	Methacholine chloride	14K20-B03-300973	2
Fagron	Methacholine chloride	15F10-B02-312160	1
Fagron	Methacholine chloride	15F10-B02-315523	1
Fagron	Methacholine chloride	15F10-B02-315831	1
Fagron	Methacholine chloride	160004A	1
Fagron	Methacholine chloride	16L20-B01	1
Fagron	Methacholine chloride	16L20-B01-329970	1
Fagron	Methacholine chloride	17D13-B04	1
Fagron	Methacholine chloride	17D13-B04-334377	2
Fagron	Methacholine chloride	17D13-B04-334378	1
Fagron	Methacholine chloride	17D13-B04-340803	1
Fagron	Methacholine chloride	17H03-B02-346563	3
Fagron	Methacholine chloride	17h03-b02-346564	1
Fagron	Methacholine chloride	17H03-B02-346564	7
Fagron	Methacholine chloride	19H07-B04365767	1
Fagron	Methacholine chloride	19H07-B04-365768	2
Fagron	Methacholine chloride	19H07-B08-365767	1
Fagron	Methacholine chloride	24061503	1
Fagron	Methacholine chloride	312160	1
Flamma s.p.a	Methacholine chloride	14G30-B03-296211	1
Inresa	Methacholine chloride	160P02A/09062017	1
L12	Methacholine chloride	16329901	2
Phoenix/Cealo	Methacholine chloride	16L20-B01-329968	1

- 236 021 spectra from 1515 *Apo-Ident* customers from a total of 49 226 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Methacholine chloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Methacholine chloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	520	0	152 442
Type B	0	270	0	201 814
Type C	0	46	0	236 021

The substance/substance group *Methacholine chloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8462 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.7778 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 86.9565 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20733	20733	0.00	211.67
21251	20733	24.46	196.09
21420	25249	86.66	185.92
21590	22635	17.45	205.96
21592	20733	27.17	185.84
22635	22635	0.00	224.30
22661	20733	26.77	199.83
22662	22635	11.02	209.88
22976	20733	7.75	212.64
22977	20733	25.07	203.76
25249	25249	0.00	211.68

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Methionine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20971-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Methionine; Methioninum

Special notes

When selecting the *Methionine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Methionine	6	9	1

Second-stage model

For differentiation of the substance/substance group *Methionine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Methionine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ornithine aspartate	96.16	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Methionine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Methionine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Methionine	1602012	22368	60	20160219*
Euro OTC	Methionine	2011016	25469	40	20201130*
Euro OTC	Methionine	2108013	25763	50	20210902*
Fagron	Methionine	12K01-N03	20971	40	1402432
Fagron	Methionine	13L19-B36-295115	21786	60	20140108
Fagron	Methionine	19L20-F03-370997	25747	50	20200213

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 300 spectra of 6 reference samples from the substance/substance group *Methionine*. These

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 662 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 410 spectra of 12 reference samples from the substance/substance group *Methionine*.
- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Methionine	1609024	22787	40
Euro OTC	Methionine	1703042	23126	40
Euro OTC	Methionine	1710008	23777	40
Euro OTC	Methionine	1904012	24674	40
Euro OTC	Methionine	1909004	24851	40
Euro OTC	Methionine	2205001	26194	40
Euro OTC	Methionine	2301004	26529	40
Euro OTC	Methionine	2305026	26769	30
Fagron	Methionine	23A16-B02-226111	26635	40
Euro OTC	Methionine	2205001	26194SI	20
Euro OTC	Methionine	2301004	26529SI	20
Fagron	Methionine	23A16-B02-226111	26635SI	20

- 201 674 spectra from a total of 4036 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Methionine*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Fagron	Methionine	21A08-F04-376464	1

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Methionine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Methionine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	410	0	201 674
Type C	0	1	0	236 066

The substance/substance group *Methionine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.5366 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20971	20971	0.00	189.65
21786	22368	7.53	188.60
22368	22368	0.00	190.99
25469	25469	0.00	190.24
25747	25763	11.04	189.07
25763	25763	0.00	189.75

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Methoxsalen**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20233-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Methoxsalen; Methoxsalenum

Special notes

When selecting the *Methoxsalen* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Methoxsalen	8	11	106

Second-stage model

For differentiation of the substance/substance group *Methoxsalen* the following second-stage model is used:

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Methoxsalen* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	123.60	–
⋮	⋮	⋮
Ciprofloxacin hydrochloride	>50	279.44
Sodium citrate	>50	285.81
Capsaicin	>50	330.66
Prednicarbate	>50	341.86
Levocarnitine	>50	353.46
Quinine hydrochloride dihydrate	>50	371.98
Oxybutynin hydrochloride	>50	383.04
Cyproterone acetate	>50	427.61
Triclosan	>50	439.07
Pyridoxal-5-phosphate	>50	465.80
Heparin sodium	>50	674.37
Tetracaine	>50	691.06
Amitriptyline hydrochloride	>50	898.43
Alfatradiol	>50	956.29
Valine	>50	998.36
Norethisterone acetate	>50	1316.79
Sucrose	>50	2025.22
Amifampridine	>50	2149.98

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Methoxsalen* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Methoxsalen*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Methoxsalen	16103003	23167	40	20160415
Caelo	Methoxsalen	170781	23333	40	20170427*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Methoxsalen	170781	23346	40	20170427*
Euro OTC	Methoxsalen	130604101	21555	60	20130805
Euro OTC	Methoxsalen	1506013	21862	60	20150706*
Euro OTC	Methoxsalen	1608019	22785	40	20160913*
Euro OTC	Methoxsalen	2106002	25702	50	20210623*
Fagron	Methoxsalen	15J15-B03-321321	23165	40	20151124
Fagron	Methoxsalen	18A12-B50-355102	24697	40	20181112

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 410 spectra of 9 reference samples from the substance/substance group *Methoxsalen*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 552 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 480 spectra of 15 reference samples from the substance/substance group *Methoxsalen*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Methoxsalen	16103014	23166	40
Caelo	Methoxsalen	191960	24760	40
Caelo	Methoxsalen	22000545003	26312	30
Caelo	Methoxsalen	24001655	27312	30
Euro OTC	Methoxsalen	1802021	24070	40
Euro OTC	Methoxsalen	1904009	24774	40
Euro OTC	Methoxsalen	2006025	25319	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Methoxsalen	2002046	25353	40
Euro OTC	Methoxsalen	2211015	26528	40
Euro OTC	Methoxsalen	2406012	27397	40
Fagron	Methoxsalen	22D19-B01-218575	26291	30
Caelo	Methoxsalen	22000545003	26312SI	20
Euro OTC	Methoxsalen	2106002	25702SI[†]	10
Euro OTC	Methoxsalen	2211015	26528SI	20
Fagron	Methoxsalen	22D19-B01-218575	26291SI	20

- 201 604 spectra from a total of 4033 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 388 spectra from 205 *Apo-Ident* customers from 111 batches from the substance/substance group *Methoxsalen*.

- Among them are spectra of independent samples from 106 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Methoxsalen	2106002-01	2
	Methoxsalen	22003782004	1
	Methoxsalen	2211015-01	3
AHD	Methoxsalen	15244204	1
AHD	Methoxsalen	1608019-02	1
AHD	Methoxsalen	16103019	1
AHD	Methoxsalen	17078101	1
AHD	Methoxsalen	17078108	2
Anzag	Methoxsalen	1306041-01	1
Anzag	Methoxsalen	2211015-01	1
Anzag	Methoxsalen	APHCFMPC16011M	1
Apo-ident/Alliance	Methoxsalen	1802021-01	1
Audor Pharma	Methoxsalen	1203009M	1
Audor Pharma	Methoxsalen	15244213	1
Audor Pharma	Methoxsalen	AP1011024-01M	1
Audor Pharma	Methoxsalen	AP15244213M	6
Audor Pharma	Methoxsalen	APHCFMPC16011M	6
Audor Pharma	Methoxsalen	APHCFMPC18003M	3
Bombastus	Methoxsalen	15J15-B03-336704	1
Caelo	Methoxsalen	1136428	1
Caelo	Methoxsalen	11376413	2
Caelo	Methoxsalen	11376420	1
Caelo	Methoxsalen	11376433	1
Caelo	Methoxsalen	1409003-01	5
Caelo	Methoxsalen	1409003-02	1
Caelo	Methoxsalen	14F06-B05-296501	1
Caelo	Methoxsalen	1503009-01	2

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Methoxsalen	150613-01	1
Caelo	Methoxsalen	15099802	1
Caelo	Methoxsalen	15244204	3
Caelo	Methoxsalen	15244205	2
Caelo	Methoxsalen	15244209	1
Caelo	Methoxsalen	15244211	1
Caelo	Methoxsalen	15244216	1
Caelo	Methoxsalen	16/079/M	1
Caelo	Methoxsalen	1608019-02	2
Caelo	Methoxsalen	16103004	1
Caelo	Methoxsalen	16103008	1
Caelo	Methoxsalen	17078101	2
Caelo	Methoxsalen	17078107	1
Caelo	Methoxsalen	17078108	3
Caelo	Methoxsalen	17078114	2
Caelo	Methoxsalen	1802021-01	3
Caelo	Methoxsalen	18A12-B50-354863	1
Caelo	Methoxsalen	190441001	1
Caelo	Methoxsalen	190441002	3
Caelo	Methoxsalen	19044103	5
Caelo	Methoxsalen	19044107	2
Caelo	Methoxsalen	190441074	1
Caelo	Methoxsalen	19044108	1
Caelo	Methoxsalen	19044110	7
Caelo	Methoxsalen	1904411002	1
Caelo	Methoxsalen	191960003	1
Caelo	Methoxsalen	191960006	2
Caelo	Methoxsalen	191960008	1
Caelo	Methoxsalen	191960009	3
Caelo	Methoxsalen	19196001	2
Caelo	Methoxsalen	20002295002	3
Caelo	Methoxsalen	20002295003	1
Caelo	Methoxsalen	20002295004	1
Caelo	Methoxsalen	20002295006	2
Caelo	Methoxsalen	20002295010	1
Caelo	Methoxsalen	20002295012	2
Caelo	Methoxsalen	2002046-01	1
Caelo	Methoxsalen	22000545001	1
Caelo	Methoxsalen	22000545003	1
Caesar & Loretz GmbH...	Methoxsalen	20002295003	1
Caesar & Loretz GmbH	Methoxsalen	190441001	1
Caesar & Loretz GmbH	Methoxsalen	19044103	2
Caesar & Loretz GmbH	Methoxsalen	19044108	1
Caesar & Loretz GmbH	Methoxsalen	19044110	2
Caesar & Loretz GmbH	Methoxsalen	20002295003	1
Caesar & Loretz GmbH	Methoxsalen	20002295007	2
Caesar&Lorenz	Methoxsalen	20002295003	1
EU.RHO.Pharm	Methoxsalen	2006025-02	2
EuRho/ AHD	Methoxsalen	16103019	1
EuRho/ Phoenix	Methoxsalen	2106002-01	2
EuRho/Fiebig	Methoxsalen	1802021-01	1
EuRho/VDL	Methoxsalen	1608019-02	1
EuRho	Methoxsalen	1104010-01	1
EuRho	Methoxsalen	2106002-01	2
Euro OCT	Methoxsalen	1802021-01	1
Euro OCT	Methoxsalen	1904009-01	1
Euro OCT	Methoxsalen	1904009-02	1
Euro OTC	Methoxsalen	1104010-01	1
Euro OTC	Methoxsalen	1108019-01	1
Euro OTC	Methoxsalen	1203009-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Methoxsalen	120901501	1
Euro OTC	Methoxsalen	1209015-01	4
Euro OTC	Methoxsalen	130604101	1
Euro OTC	Methoxsalen	1306041-01	5
Euro OTC	Methoxsalen	1409003-01	5
Euro OTC	Methoxsalen	140900302	1
Euro OTC	Methoxsalen	1409003-02	3
Euro OTC	Methoxsalen	150300901	1
Euro OTC	Methoxsalen	1503009-01	12
Euro OTC	Methoxsalen	1503009-02	9
Euro OTC	Methoxsalen	1506013_01	1
Euro OTC	Methoxsalen	1506013-01	19
Euro OTC	Methoxsalen	1506013-02	7
Euro OTC	Methoxsalen	1608019	1
Euro OTC	Methoxsalen	1608019-01	4
Euro OTC	Methoxsalen	160801902	1
Euro OTC	Methoxsalen	1608019-02	18
Euro OTC	Methoxsalen	1608019-1	1
Euro OTC	Methoxsalen	1802021/01	1
Euro OTC	Methoxsalen	1802021-01	40
Euro OTC	Methoxsalen	1904009-01	25
Euro OTC	Methoxsalen	1904009-02	1
Euro OTC	Methoxsalen	2006025-01	4
Euro OTC	Methoxsalen	2006025-02	1
Euro OTC	Methoxsalen	2106002-01	13
Euro/Phönix	Methoxsalen	1608019-02	1
Euroo	Methoxsalen	1503009-01	1
Fag	Methoxsalen	20f-12-F01	1
Fagron	Methoxsalen	11D07-N16	1
Fagron	Methoxsalen	11f21-n02	1
Fagron	Methoxsalen	11F21-N02	1
Fagron	Methoxsalen	12E02-N05	2
Fagron	Methoxsalen	12G02-N14	1
Fagron	Methoxsalen	14f06-b05-296500	1
Fagron	Methoxsalen	14F06-B05-296500	1
Fagron	Methoxsalen	14F06-B05-296501	2
Fagron	Methoxsalen	14F06-B05-301978	1
Fagron	Methoxsalen	150601301	1
Fagron	Methoxsalen	15C10-B99-306266	1
Fagron	Methoxsalen	15F23-B03	1
Fagron	Methoxsalen	15F23-B03-309644	1
Fagron	Methoxsalen	15F23-B03-316262	1
Fagron	Methoxsalen	15F23-B03-318166	5
Fagron	Methoxsalen	15J15-B03-321321	1
Fagron	Methoxsalen	15J15-B03-341859	1
Fagron	Methoxsalen	18A12-B50-359351	1
Fagron	Methoxsalen	19H05-B02-366102	1
Fagron	Methoxsalen	21111814	1
Fagron	Methoxsalen	2111A-03262	2
Fagron	Methoxsalen	B02-3661001	1
Fagron	Methoxsalen	MS01/13-14	1
Franco / Ebert	Methoxsalen	CMX-15/12	1
Herbal Creations/AHD	Methoxsalen	APHCFMPC16011M	1
Herbal Creations/Cae…	Methoxsalen	15244203	1
Herbal Creations/Cae…	Methoxsalen	15244205	1
Herbal creations/Cae…	Methoxsalen	15244208	1
Herbal creations/Cae…	Methoxsalen	15244212	1
Herbal Creations	Methoxsalen	1608019-01	1
L10	Methoxsalen	2106002-01	2
Nachprüfung	Methoxsalen	4211Q-03262	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Methoxsalen	11D07-N16	2
Noweda	Methoxsalen	140900302	1
Noweda	Methoxsalen	19044103	2
Noweda	Methoxsalen	2006025-01	1
Noweda	Methoxsalen	2211015-01	1
PHOENIX 18.02.14	Methoxsalen	1306041-01	2
Phoenix	Methoxsalen	14F06-B05-296502	1
Phönix	Methoxsalen	1608019-01	1
Phönix	Methoxsalen	1608019-02	1
Phönix	Methoxsalen	1802021-01	1
Phytoceut.Ltd	Methoxsalen	1503009-01	3
Sanacorp	Methoxsalen	1AKD6	1
Say Phytoceut. Ltd	Methoxsalen	1209015-01	3

- 235 679 spectra from 1515 *Apo-Ident* customers from a total of 49 147 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Methoxsalen* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Methoxsalen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	410	0	152 552
Type B	0	480	0	201 604
Type C	0	387	1	235 679

The substance/substance group *Methoxsalen* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5366 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.7500 %)
Type C	100.0000 % (> 99.9007 %)	99.7423 % (> 98.9691 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested

reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21555	21862	6.83	221.52
21862	21862	0.00	238.08
22785	22785	0.00	234.59
23165	21862	10.68	217.89
23167	21862	12.21	213.72
23333	23333	0.00	214.05
23346	23346	0.00	209.04
24697	21862	10.54	218.18
25702	25702	0.00	205.99

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Methyl-4-hydroxybenzoate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20345-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Methyl-4-hydroxybenzoate; Methylis parahydroxybenzoas

Special notes

When selecting the *Methyl-4-hydroxybenzoate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Methyl-4-hydroxybenzoate	6	18	139

Second-stage model

For differentiation of the substance/substance group *Methyl-4-hydroxybenzoate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Methyl-4-hydroxybenzoate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	104.35	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Methyl-4-hydroxybenzoate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Methyl-4-hydroxybenzoate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Methyl-4-hydroxybenzoate	11090034	20693	40	20110428
Caelo	Methyl-4-hydroxybenzoate	181769	24223	40	20180824*
Euro OTC	Methyl-4-hydroxybenzoate	1205025-01	20697	40	20120601
Euro OTC	Methyl-4-hydroxybenzoate	1601037	22305	60	20160119*
Fagron	Methyl-4-hydroxybenzoate	14L30-T01-018345	23223	40	20150309
Fagron	Methyl-4-hydroxybenzoate	19B05-T03-062158	24588	40	20190228

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 260 spectra of 6 reference samples from the substance/substance group *Methyl-4-hydroxybenzoate*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 790 spectra of 21 reference samples from the substance/substance group *Methyl-4-hydroxybenzoate*.
- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Methyl-4-hydroxybenzoate	13268813	21439	60
Caelo	Methyl-4-hydroxybenzoate	15063820	23216	40
Caelo	Methyl-4-hydroxybenzoate	171581	23317	40
Caelo	Methyl-4-hydroxybenzoate	191302	24711	40
Caelo	Methyl-4-hydroxybenzoate	192334	24886	40
Caelo	Methyl-4-hydroxybenzoate	22000388	26117	40
Caelo	Methyl-4-hydroxybenzoate	22003498	26475	40
Caelo	Methyl-4-hydroxybenzoate	23000896	26852	40
Caelo	Methyl-4-hydroxybenzoate	23003474	27102	40
Euro OTC	Methyl-4-hydroxybenzoate	1706005	23703	40
Euro OTC	Methyl-4-hydroxybenzoate	1807009	24148	40
Euro OTC	Methyl-4-hydroxybenzoate	1902025	24568	40
Euro OTC	Methyl-4-hydroxybenzoate	1909009	24852	40
Euro OTC	Methyl-4-hydroxybenzoate	2004013	25155	40
Euro OTC	Methyl-4-hydroxybenzoate	2010001	25409	40
Euro OTC	Methyl-4-hydroxybenzoate	2304023	26639	40
Fagron	Methyl-4-hydroxybenzoate	22L02-B13-226168	26548	40
Gatt-Koller	Methyl-4-hydroxybenzoate	23J00964	27100	30
Caelo	Methyl-4-hydroxybenzoate	22000388	26117SI	20
Caelo	Methyl-4-hydroxybenzoate	22003498	26475SI	20
Fagron	Methyl-4-hydroxybenzoate	22L02-B13-226168	26548SI	20

- 201 294 spectra from a total of 4027 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information

provided by the customer regarding manufacturer and batch number.

- 694 spectra from 475 *Apo-Ident* customers from 141 batches from the substance/substance group *Methyl-4-hydroxybenzoate*.
- Among them are spectra of independent samples from 136 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Methyl-4-hydroxybenzoate	2010001-02	4
	Methyl-4-hydroxybenzoate	22000388006	1
	Methyl-4-hydroxybenzoate	22000388010	1
	Methyl-4-hydroxybenzoate	22003498003	11
	Methyl-4-hydroxybenzoate	22J02568	1
	Methyl-4-hydroxybenzoate	23000896007	1
AHD	Methyl-4-hydroxybenzoate	12251624	1
AHD	Methyl-4-hydroxybenzoate	17158101	1
AHD	Methyl-4-hydroxybenzoate	17343002	1
AHD	Methyl-4-hydroxybenzoate	22003498003	1
AHD	Methyl-4-hydroxybenzoate	2300896007	1
Anzag	Methyl-4-hydroxybenzoate	11345115	1
apo-ident	Methyl-4-hydroxybenzoate	1706005-01	1
Bombastus	Methyl-4-hydroxybenzoate	1212011-01	1
Caelo	Methyl-4-hydroxybenzoate		2
Caelo	Methyl-4-hydroxybenzoate	1000076005	1
Caelo	Methyl-4-hydroxybenzoate	1108211930	1
Caelo	Methyl-4-hydroxybenzoate	11090003	1
Caelo	Methyl-4-hydroxybenzoate	11090030	1
Caelo	Methyl-4-hydroxybenzoate	11090031	4
Caelo	Methyl-4-hydroxybenzoate	111003301	1
Caelo	Methyl-4-hydroxybenzoate	11345103	1
Caelo	Methyl-4-hydroxybenzoate	11345115	7
Caelo	Methyl-4-hydroxybenzoate	11345120	2
Caelo	Methyl-4-hydroxybenzoate	12081502	1
Caelo	Methyl-4-hydroxybenzoate	12251605	2
Caelo	Methyl-4-hydroxybenzoate	12251611	1
Caelo	Methyl-4-hydroxybenzoate	12251619	1
Caelo	Methyl-4-hydroxybenzoate	12251624	5
Caelo	Methyl-4-hydroxybenzoate	1251624	1
Caelo	Methyl-4-hydroxybenzoate	13081308	1
Caelo	Methyl-4-hydroxybenzoate	13268802	1
Caelo	Methyl-4-hydroxybenzoate	13268803	1
Caelo	Methyl-4-hydroxybenzoate	13268804	9
Caelo	Methyl-4-hydroxybenzoate	13268809	5
Caelo	Methyl-4-hydroxybenzoate	13268813	7
Caelo	Methyl-4-hydroxybenzoate	13268815	1
Caelo	Methyl-4-hydroxybenzoate	13268819	1
Caelo	Methyl-4-hydroxybenzoate	13268821	1
Caelo	Methyl-4-hydroxybenzoate	14120207	1
Caelo	Methyl-4-hydroxybenzoate	14120208	5
Caelo	Methyl-4-hydroxybenzoate	15063802	8
Caelo	Methyl-4-hydroxybenzoate	15063803	1
Caelo	Methyl-4-hydroxybenzoate	15063806	8
Caelo	Methyl-4-hydroxybenzoate	15063812	3
Caelo	Methyl-4-hydroxybenzoate	15063813	2
Caelo	Methyl-4-hydroxybenzoate	15063818	4
Caelo	Methyl-4-hydroxybenzoate	15063819	4
Caelo	Methyl-4-hydroxybenzoate	15063819/1210217	1
Caelo	Methyl-4-hydroxybenzoate	15063820	4
Caelo	Methyl-4-hydroxybenzoate	15222203	5
Caelo	Methyl-4-hydroxybenzoate	15298101	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Methyl-4-hydroxybenzoate	15298102	12
Caelo	Methyl-4-hydroxybenzoate	15444905	1
Caelo	Methyl-4-hydroxybenzoate	15444911	1
Caelo	Methyl-4-hydroxybenzoate	15444913	4
Caelo	Methyl-4-hydroxybenzoate	15444916	1
Caelo	Methyl-4-hydroxybenzoate	1601037-01	6
Caelo	Methyl-4-hydroxybenzoate	16256103	6
Caelo	Methyl-4-hydroxybenzoate	16256104	2
Caelo	Methyl-4-hydroxybenzoate	16256114	1
Caelo	Methyl-4-hydroxybenzoate	16256115	2
Caelo	Methyl-4-hydroxybenzoate	16256117	2
Caelo	Methyl-4-hydroxybenzoate	16256118	6
Caelo	Methyl-4-hydroxybenzoate	17158101	27
Caelo	Methyl-4-hydroxybenzoate	17343002	14
Caelo	Methyl-4-hydroxybenzoate	17343009	2
Caelo	Methyl-4-hydroxybenzoate	17343010	9
Caelo	Methyl-4-hydroxybenzoate	17343013	20
Caelo	Methyl-4-hydroxybenzoate	1807009-01	1
Caelo	Methyl-4-hydroxybenzoate	1816903	1
Caelo	Methyl-4-hydroxybenzoate	18176903	27
Caelo	Methyl-4-hydroxybenzoate	18176910	15
Caelo	Methyl-4-hydroxybenzoate	18176919	2
Caelo	Methyl-4-hydroxybenzoate	190672106	1
Caelo	Methyl-4-hydroxybenzoate	191302001	36
Caelo	Methyl-4-hydroxybenzoate	191302002	3
Caelo	Methyl-4-hydroxybenzoate	191302003	7
Caelo	Methyl-4-hydroxybenzoate	19130203	6
Caelo	Methyl-4-hydroxybenzoate	19130205	19
Caelo	Methyl-4-hydroxybenzoate	1913022001	1
Caelo	Methyl-4-hydroxybenzoate	19132001	1
Caelo	Methyl-4-hydroxybenzoate	2000388006	1
Caelo	Methyl-4-hydroxybenzoate	21000076005	18
Caelo	Methyl-4-hydroxybenzoate	21000076005n	1
Caelo	Methyl-4-hydroxybenzoate	21000076007	1
Caelo	Methyl-4-hydroxybenzoate	21000076011	17
Caelo	Methyl-4-hydroxybenzoate	21000076015	10
Caelo	Methyl-4-hydroxybenzoate	21000076017	1
Caelo	Methyl-4-hydroxybenzoate	22000388006	15
Caelo	Methyl-4-hydroxybenzoate	22000388009	2
Caelo	Methyl-4-hydroxybenzoate	22003498003	1
Caelo	Methyl-4-hydroxybenzoate	220830(22000388006)	1
Caelo	Methyl-4-hydroxybenzoate	22092002	1
Caelo	Methyl-4-hydroxybenzoate	290114PML01	1
Caelo	Methyl-4-hydroxybenzoate	6091402	1
Caelo	Methyl-4-hydroxybenzoate	713Q-01930	1
Caelo	Methyl-4-hydroxybenzoate	79/19	1
Caelo	Methyl-4-hydroxybenzoate	9011303	1
Caelo	Methyl-4-hydroxybenzoate	Caelo	1
Caesar & Loretz GmbH...	Methyl-4-hydroxybenzoate	22000388006	1
Caesar & Loretz GmbH...	Methyl-4-hydroxybenzoate	19130205	1
Caesar & Loretz GmbH/Gehe	Methyl-4-hydroxybenzoate	21000076015	1
Caesar & Loretz GmbH/Kehr	Methyl-4-hydroxybenzoate	191302003	1
Caesar & Loretz GmbH...	Methyl-4-hydroxybenzoate	191302001	1
Caesar & Loretz GmbH...	Methyl-4-hydroxybenzoate	18176903	1
Caesar & Loretz GmbH...	Methyl-4-hydroxybenzoate	191302003	1
Caesar & Loretz GmbH...	Methyl-4-hydroxybenzoate	19130203	1
Caesar & Loretz GmbH...	Methyl-4-hydroxybenzoate	21000076005	2
Caesar & Loretz GmbH...	Methyl-4-hydroxybenzoate	21000076005	1
Caesar & Loretz GmbH/Sa	Methyl-4-hydroxybenzoate	19130205	1
Caesar & Loretz GmbH...	Methyl-4-hydroxybenzoate	21000076005	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Methyl-4-hydroxybenzoate	21000076011	1
Caesar & Loretz GmbH	Methyl-4-hydroxybenzoate	13268809	1
Caesar & Loretz GmbH	Methyl-4-hydroxybenzoate	17158101	1
Caesar & Loretz GmbH	Methyl-4-hydroxybenzoate	18176903	3
Caesar & Loretz GmbH	Methyl-4-hydroxybenzoate	18176910	6
Caesar & Loretz GmbH	Methyl-4-hydroxybenzoate	191302001	8
Caesar & Loretz GmbH	Methyl-4-hydroxybenzoate	191302003	6
Caesar & Loretz GmbH	Methyl-4-hydroxybenzoate	19130205	5
Caesar & Loretz GmbH	Methyl-4-hydroxybenzoate	21000076005	9
Caesar & Loretz GmbH	Methyl-4-hydroxybenzoate	21000076011	2
Caesar & Loretz GmbH	Methyl-4-hydroxybenzoate	21000076015	4
Caesar & Loretz GmbH	Methyl-4-hydroxybenzoate	220003388006	1
Caesar & Loretz GmbH	Methyl-4-hydroxybenzoate	22000388006	6
Caesar & Loretz GmbH	Methyl-4-hydroxybenzoate	22000388009	1
Caesar & Loretz GmbH	Methyl-4-hydroxybenzoate	22003498003	1
Caesar & Loretz Hild...	Methyl-4-hydroxybenzoate	191302003	1
Caesar & Loretz/Noweda	Methyl-4-hydroxybenzoate	191302001	1
Caesar & Loretz	Methyl-4-hydroxybenzoate	17343002	1
Caesar&loretz,Phoenix	Methyl-4-hydroxybenzoate	13268821	1
Caesar&Loretz	Methyl-4-hydroxybenzoate	17158101	1
Caesar/Noweda	Methyl-4-hydroxybenzoate	15063806	1
Cealo/Anzag	Methyl-4-hydroxybenzoate	19130205	1
Cealo/Gehe	Methyl-4-hydroxybenzoate	16256104	1
Eigenherstellung	Methyl-4-hydroxybenzoate		1
Eigenherstellung	Methyl-4-hydroxybenzoate	100912PML01	1
EuRho/ NOWEDA	Methyl-4-hydroxybenzoate	EA2781	1
EuRho	Methyl-4-hydroxybenzoate	110403101	1
Euro OTC	Methyl-4-hydroxybenzoate	1009022-01	1
Euro OTC	Methyl-4-hydroxybenzoate	1212011-01	1
Euro OTC	Methyl-4-hydroxybenzoate	1401027-01	1
Euro OTC	Methyl-4-hydroxybenzoate	1401027-02	2
Euro OTC	Methyl-4-hydroxybenzoate	140600501	1
Euro OTC	Methyl-4-hydroxybenzoate	1406005-01	2
Euro OTC	Methyl-4-hydroxybenzoate	1502009-01	11
Euro OTC	Methyl-4-hydroxybenzoate	1507042-01	10
Euro OTC	Methyl-4-hydroxybenzoate	1507042-02	4
Euro OTC	Methyl-4-hydroxybenzoate	1601037	1
Euro OTC	Methyl-4-hydroxybenzoate	1601037-01	5
Euro OTC	Methyl-4-hydroxybenzoate	1706005-01	9
Euro OTC	Methyl-4-hydroxybenzoate	1706005-02	3
Euro OTC	Methyl-4-hydroxybenzoate	170605-01	1
Euro OTC	Methyl-4-hydroxybenzoate	172620	1
Euro OTC	Methyl-4-hydroxybenzoate	1758101	1
Euro OTC	Methyl-4-hydroxybenzoate	1807009-01	28
Euro OTC	Methyl-4-hydroxybenzoate	1902025-01	3
Euro OTC	Methyl-4-hydroxybenzoate	19090009-01	1
Euro OTC	Methyl-4-hydroxybenzoate	1909009-01	8
Euro OTC	Methyl-4-hydroxybenzoate	2004013/01	1
Euro OTC	Methyl-4-hydroxybenzoate	200401301	2
Euro OTC	Methyl-4-hydroxybenzoate	2004013-01	5
Euro OTC	Methyl-4-hydroxybenzoate	2010001-01	3
Euro OTC	Methyl-4-hydroxybenzoate	2010001-02	5
Euro OTC	Methyl-4-hydroxybenzoate	2606022	1
Euro OTC	Methyl-4-hydroxybenzoate	2717M-01930	1
Euro OTC	Methyl-4-hydroxybenzoate	280903701	2
Euro OTC	Methyl-4-hydroxybenzoate	3115M-01930	1
Euro OTC	Methyl-4-hydroxybenzoate	3518A-01930	1
Euro OTC	Methyl-4-hydroxybenzoate	4312I-01930	1
Euro OTC	Methyl-4-hydroxybenzoate	4314U-01930	1
Euro OTC	Methyl-4-hydroxybenzoate	EA2781	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro/Phönix	Methyl-4-hydroxybenzoate	201000101	1
Fagron	Methyl-4-hydroxybenzoate		1
Fagron	Methyl-4-hydroxybenzoate	12D18-N01	1
Fagron	Methyl-4-hydroxybenzoate	12H02-N08	1
Fagron	Methyl-4-hydroxybenzoate	13B25-N03	2
Fagron	Methyl-4-hydroxybenzoate	13E27-N09	1
Fagron	Methyl-4-hydroxybenzoate	16256115	1
Fagron	Methyl-4-hydroxybenzoate	20111125-1	1
GATT-KOLLER/PHOENIX	Methyl-4-hydroxybenzoate	6112/01142814	1
Gatt-Koller	Methyl-4-hydroxybenzoate	1803308	1
Gehe	Methyl-4-hydroxybenzoate	11090020	1
Gehe	Methyl-4-hydroxybenzoate	11090031	1
Gehe	Methyl-4-hydroxybenzoate	15063818	1
Gehe	Methyl-4-hydroxybenzoate	17158101	1
Gehe	Methyl-4-hydroxybenzoate	1902025-01	1
Gehe	Methyl-4-hydroxybenzoate	2010001-02	1
Geibo	Methyl-4-hydroxybenzoate	22000388006	1
Hänseler	Methyl-4-hydroxybenzoate		2
Jenne	Methyl-4-hydroxybenzoate	21000076015	1
Kehr	Methyl-4-hydroxybenzoate	22003498003	1
L30	Methyl-4-hydroxybenzoate	17158101	2
Nachprüfung vom 31.1...	Methyl-4-hydroxybenzoate	12251624	2
Nachprüfung	Methyl-4-hydroxybenzoate	1718M-01930	1
Noweda/Caesar & Lore...	Methyl-4-hydroxybenzoate	22000388009	1
Noweda	Methyl-4-hydroxybenzoate	16256118	1
Noweda	Methyl-4-hydroxybenzoate	1706005-02	1
Noweda	Methyl-4-hydroxybenzoate	17158101	1
Noweda	Methyl-4-hydroxybenzoate	191302003	1
Phoenix	Methyl-4-hydroxybenzoate	1706005-01	1
Phoenix	Methyl-4-hydroxybenzoate	18176910	1
Phoenix	Methyl-4-hydroxybenzoate	200046011	1
Phoenix	Methyl-4-hydroxybenzoate	21000076011	1
Phoenix	Methyl-4-hydroxybenzoate	2100076007	1
Phoenix	Methyl-4-hydroxybenzoate	22000388009	1
Phoenix	Methyl-4-hydroxybenzoate	22003498003	1
Phönix 14.01.2014	Methyl-4-hydroxybenzoate	12251624	1
phönix 4.12.2013	Methyl-4-hydroxybenzoate	1212011/01	1
PHÖNIX	Methyl-4-hydroxybenzoate	15063819	1
Phönix	Methyl-4-hydroxybenzoate	16256103	1
Phönix	Methyl-4-hydroxybenzoate	17343010	1
Phönix	Methyl-4-hydroxybenzoate	1807009-01	1
Phönix	Methyl-4-hydroxybenzoate	191302001	1
Phönix	Methyl-4-hydroxybenzoate	2010001-01	2
Phönix	Methyl-4-hydroxybenzoate	2AKD3	1
sanacorb	Methyl-4-hydroxybenzoate	17343010	1
Sanacorp E.K :2,76...	Methyl-4-hydroxybenzoate	13268804	1

- 235 373 spectra from 1515 *Apo-Ident* customers from a total of 49 119 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Methyl-4-hydroxybenzoate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Methyl-4-hydroxybenzoate*

and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	790	0	201 294
Type C	0	685	9	235 373

The substance/substance group *Methyl-4-hydroxybenzoate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2405 %)
Type C	100.0000 % (> 99.9007 %)	98.7032 % (> 98.2709 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20693	22305	10.68	200.51
20697	22305	11.52	200.96
22305	22305	0.00	203.35
23223	22305	12.97	201.26
24223	24223	0.00	200.76
24588	22305	15.83	203.83

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Methylcellulose**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20705-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Methylcellulose; Hydroxypropylcellulose; Hydroxypropylcellulosum; Hypromellose; Hypromellosum; Methylcellulosum

Special notes

When selecting the *Methylcellulose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Methylcellulose	24	16	251

Second-stage model

For differentiation of the substance/substance group *Methylcellulose* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Methylcellulose* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prednisolon dihydrogen phosphate di...	92.76	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Methylcellulose* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Methylcellulose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Hydroxypropylcellulose	12093107	20686	40	1402049
Caelo	Hydroxypropylcellulose	14189804	21767	60	AR-15-FG-014922-01
Caelo	Hydroxypropylcellulose	15345001	22258	60	20151104
Caelo	Hydroxypropylcellulose	181146	24249	40	20180618*
Caelo	Hydroxypropylcellulose	20000942007	25426	40	20200505
Caelo	Hydroxypropylcellulose	21001994001	25981	40	20211004
Caelo	Hydroxypropylcellulose	21001994001	25981SI	30	20211004
Caelo	Hydroxypropylcellulose	22003732	26721	40	20230124*
Caelo	Hydroxypropylcellulose	22003732	26721SI	20	20230124*
Caelo	Hydroxypropylcellulose	24000194	27139	40	20240322*
Caelo	Hydroxypropylcellulose	24000194	27139SI	20	20240322*
Caelo	Hypromellose	13155006	20919	40	1402056
Caelo	Hypromellose	13155006	20931	40	20130529
Caelo	Hypromellose	14338801	21702	45	20141217
Caelo	Hypromellose	192852	25230	40	20191220*
Caelo	Hypromellose	20000987	25231	40	20200518*
Caelo	Hypromellose	21001141	26148	40	20210729*
Caelo	Hypromellose	22003524	26488	40	20221220*
Caelo	Hypromellose	22003524	26488SI	20	20221220*
Fagron	Hypromellose	15G08-B14-314845	22609	40	20150727
Fagron	Hypromellose	19G17-B04-194255	25060	40	20190830
Fagron	Hypromellose	22B26-B10-223114	26636	40	231005103

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Methylcellulose	13130115	21570	60	20130517
Caelo	Methylcellulose	160602	22457	60	20160323*
Caelo	Methylcellulose	192473	25286	40	20191202*
Caelo	Methylcellulose	20002631	25622	40	20201027*
Fagron	Methylcellulose	12D02-N09	20705	40	1402447
Fagron	Methylcellulose	15H04-B07-331291	23224	40	20150824
Fagron	Methylcellulose	18D03-B05-361882	25188	40	20180507

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1175 spectra of 29 reference samples from the substance/substance group *Methylcellulose*. These samples are listed above in the *calibration samples* section. The reference samples come from 24 different batches.
- 151 787 spectra from a total of 2818 batches from further 481 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 770 spectra of 21 reference samples from the substance/substance group *Methylcellulose*.
- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hydroxypropylcellulose	15345009	23123	40
Caelo	Hydroxypropylcellulose	17355801	23974	40
Caelo	Hypromellose	162244	22757	40
Caelo	Hypromellose	171150	23284	40
Caelo	Hypromellose	190696	24516	40
Caelo	Hypromellose	22001980	26242	40
Caelo	Hypromellose	23000497	26855	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Hypromellose	24001679	27434	40
Caelo	Methylcellulose	171704	23627	40
Caelo	Methylcellulose	183318	24560	40
Caelo	Methylcellulose	22000891	26107	40
Caelo	Methylcellulose	23001536	26975	40
Caelo	Methylcellulose	24000306	27130	40
Fagron	Methylcellulose	20E28-F04-371902	25724	50
Fagron	Methylcellulose	21F04-F05-378883	25937	40
Fagron	Methylcellulose	22K07-B14-224511	26547	40
Caelo	Hypromellose	21001141	26148SI[†]	20
Caelo	Hypromellose	22001980	26242SI	20
Caelo	Methylcellulose	22000891	26107SI	20
Fagron	Methylcellulose	21F04-F05-378883	25937SI	40
Fagron	Methylcellulose	22K07-B14-224511	26547SI	20

- 201 314 spectra from a total of 4028 batches from further 836 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1216 spectra from 568 *Apo-Ident* customers from 266 batches from the substance/substance group *Methylcellulose*.
- Among them are spectra of independent samples from 250 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Hypromellose	18004b03-348465	1
	Methylcellulose	22000891011	3
	Methylcellulose	22000891020	1
	Hypromellose	22003524002	3
	Hypromellose	22003524004	5
	Hypromellose	22003524005	1
	Hypromellose	22003524006	1
	Hypromellose	22003524007	3
	Hypromellose	23000497002	1
	Hypromellose	23000497003	10
	Methylcellulose	23001536003	2
	Hypromellose	23003602003	1
	Hypromellose	23D27-B06-227933	1
AHD	Hypromellose	16H23-B02-325994	1
AHD	Methylcellulose	192473004	1
AHD	Hypromellose	23000497003	2
Alliance Health 27.1…	Hypromellose	13D03-N03	1
Bombastus	Methylcellulose	17170405	1
Caelo	Methylcellulose		1
Caelo	Hypromellose	10004281003	1
Caelo	Methylcellulose	10247604	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Methylcellulose	12044903	2
Caelo	Methylcellulose	12044907	1
Caelo	Methylcellulose	12044917	1
Caelo	Methylcellulose	12044918	2
Caelo	Methylcellulose	12044922	2
Caelo	Methylcellulose	12044927	6
Caelo	Methylcellulose	12044931	2
Caelo	Hypromellose	12098702	1
Caelo	Hypromellose	12215504	2
Caelo	Hypromellose	12215505	1
Caelo	Hypromellose	12239502	1
Caelo	Methylcellulose	13021401	1
Caelo	Hydroxypropylcellulose	13031306	1
Caelo	Hydroxypropylcellulose	13031309	1
Caelo	Hypromellose	13100304	2
Caelo	Methylcellulose	13130104	5
Caelo	Methylcellulose	13130109	5
Caelo	Methylcellulose	13130115	6
Caelo	Methylcellulose	13130121	3
Caelo	Methylcellulose	1313019	1
Caelo	Hypromellose	13155002	1
Caelo	Hypromellose	13155004	11
Caelo	Hypromellose	13d03-n03	1
Caelo	Hydroxypropylcellulose	14189801	2
Caelo	Methylcellulose	14197502	7
Caelo	Methylcellulose	14197513	1
Caelo	Methylcellulose	14197514	9
Caelo	Hypromellose	14338801	3
Caelo	Hypromellose	14338802	1
Caelo	Hypromellose	14338803	1
Caelo	Hypromellose	14C05-B03-294708	1
Caelo	Hydroxypropylcellulose	15129707	1
Caelo	Methylcellulose	15179602	12
Caelo	Methylcellulose	15179605	8
Caelo	Hydroxypropylcellulose	15345001	3
Caelo	Hydroxypropylcellulose	15345005	1
Caelo	Hydroxypropylcellulose	15345008	1
Caelo	Hypromellose	15B02-B05-308852	1
Caelo	Hypromellose	15G08-B14-310845	1
Caelo	Hypromellose	15G08-B14-314845	3
Caelo	Methylcellulose	16060202	1
Caelo	Methylcellulose	16060206	12
Caelo	Methylcellulose	16060210	12
Caelo	Hypromellose	16224401	6
Caelo	Hypromellose	16224403	15
Caelo	Hypromellose	16224404	1
Caelo	Hypromellose	16224406	5
Caelo	Hypromellose	16224407	19
Caelo	Hypromellose	16224408	1
Caelo	Hypromellose	16224409	11
Caelo	Methylcellulose	16284003	10
Caelo	Methylcellulose	16284004	2
Caelo	Methylcellulose	16284006	11
Caelo	Methylcellulose	1628404	1
Caelo	Hypromellose	16B16-B07-321327	2
Caelo	Hypromellose	16H23-B02-325994	1
Caelo	Hypromellose	16H23-B02-332066	1
Caelo	Hypromellose	17115004	2
Caelo	Hypromellose	17115005	22
Caelo	Hypromellose	17115008	13

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hypromellose	171150085501	1
Caelo	Hypromellose	17132101	1
Caelo	Methylcellulose	17170404	6
Caelo	Methylcellulose	17170405	11
Caelo	Methylcellulose	17170406	1
Caelo	Hypromellose	180215H/17115004	1
Caelo	Methylcellulose	18045101	11
Caelo	Methylcellulose	18045103	2
Caelo	Methylcellulose	18045107	2
Caelo	Methylcellulose	18045110	1
Caelo	Methylcellulose	18045114	3
Caelo	Hydroxypropylcellulose	18114601	1
Caelo	Hydroxypropylcellulose	18114607	2
Caelo	Hypromellose	18132101	16
Caelo	Hypromellose	18132102	6
Caelo	Hypromellose	18132105	21
Caelo	Hypromellose	18132106	2
Caelo	Hypromellose	18132109	13
Caelo	Hypromellose	18132111	6
Caelo	Hypromellose	18132111/18132109	1
Caelo	Hypromellose	18132116	1
Caelo	Methylcellulose	183318002	4
Caelo	Methylcellulose	18331803	10
Caelo	Methylcellulose	18331804	1
Caelo	Methylcellulose	18331806	20
Caelo	Hypromellose	18A17-B04-345100	1
Caelo	Hypromellose	18D04-B03-350745	2
Caelo	Hypromellose	18D04-B03-355144	1
Caelo	Hypromellose	1906901	1
Caelo	Hypromellose	1906908	1
Caelo	Hypromellose	19069601	35
Caelo	Hypromellose	19069608	23
Caelo	Hypromellose	19069609	9
Caelo	Methylcellulose	192473003	6
Caelo	Methylcellulose	192473004	6
Caelo	Hypromellose	192852004	4
Caelo	Hypromellose	192852005	27
Caelo	Hypromellose	19285205	1
Caelo	Hypromellose	1969609	1
Caelo	Hypromellose	19G17-B04-194255	1
Caelo	Hypromellose	200000987004	1
Caelo	Hypromellose	200000987006	1
Caelo	Hypromellose	20000987003	8
Caelo	Hypromellose	20000987004	24
Caelo	Hypromellose	20000987006	19
Caelo	Hypromellose	20000987007	5
Caelo	Hypromellose	20000987044	1
Caelo	Methylcellulose	200014546013	1
Caelo	Hypromellose	20004281002	4
Caelo	Hypromellose	20004281003	7
Caelo	Methylcellulose	20004546004	4
Caelo	Methylcellulose	20004546008	5
Caelo	Methylcellulose	20004546009	5
Caelo	Methylcellulose	20004546013	4
Caelo	Methylcellulose	2000456009	1
Caelo	Hypromellose	2001980005	1
Caelo	Methylcellulose	20021401	1
Caelo	Hypromellose	21001141001	2
Caelo	Hypromellose	21001141002	9
Caelo	Hypromellose	21001141004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hypromellose	21001141005	7
Caelo	Hypromellose	21001141006	8
Caelo	Hypromellose	21001141009	1
Caelo	Hypromellose	210011411005	1
Caelo	Hydroxypropylcellulose	21001994001	1
Caelo	Methylcellulose	22000891002	3
Caelo	Methylcellulose	22000891007	1
Caelo	Methylcellulose	22000891011	1
Caelo	Hypromellose	22001980004	2
Caelo	Hypromellose	22001980005	24
Caelo	Hypromellose	22001980009	1
Caelo	Hypromellose	22001982225	1
Caelo	Hypromellose	22003524004	3
Caelo	Hypromellose	22003524005	2
Caelo	Hypromellose	22003524006	1
Caelo	Hypromellose	22003524007	1
Caelo	Methylcellulose	5081404	1
Caelo	Hypromellose	5121818	1
Caelo	Methylcellulose	5219Q-01882	1
Caelo	Hypromellose	D180F8Q011	1
Caesar & Loretz GmbH...	Hypromellose	16224403	1
Caesar & Loretz GmbH...	Methylcellulose	18331803	1
Caesar & Loretz GmbH...	Methylcellulose	20004546008	1
Caesar & Loretz GmbH...	Hypromellose	20000987006	1
Caesar & Loretz GmbH...	Hypromellose	21001141005	1
Caesar & Loretz GmbH/AHD	Hypromellose	19069609	1
Caesar & Loretz GmbH/AHD	Hypromellose	20000987004	2
Caesar & Loretz GmbH...	Methylcellulose	20004546004	1
Caesar & Loretz GmbH...	Hypromellose	19069601	1
Caesar & Loretz GmbH...	Hypromellose	192852005	3
Caesar & Loretz GmbH/Gehe	Hypromellose	19069601	2
Caesar & Loretz GmbH/Gehe	Hydroxypropylcellulose	20000942005	1
Caesar & Loretz GmbH/GEHE	Hydroxypropylcellulose	20000942005	1
Caesar & Loretz GmbH/Gehe	Hypromellose	20000987004	1
Caesar & Loretz GmbH/Gehe	Hypromellose	20004281003	1
Caesar & Loretz GmbH/Gehe	Methylcellulose	22000891002	2
Caesar & Loretz GmbH...	Methylcellulose	18331806	1
Caesar & Loretz GmbH...	Hypromellose	19069608	1
Caesar & Loretz GmbH...	Hypromellose	22001980004	1
Caesar & Loretz GmbH...	Hypromellose	22001980005	1
Caesar & Loretz GmbH...	Methylcellulose	17170405	1
Caesar & Loretz GmbH...	Hypromellose	19069601	1
Caesar & Loretz GmbH...	Hypromellose	19069609	2
Caesar & Loretz GmbH...	Hypromellose	21001141005	1
Caesar & Loretz GmbH...	Methylcellulose	20004546004	1
Caesar & Loretz GmbH...	Hydroxypropylcellulose	20003818001	1
Caesar & Loretz GmbH/Sana	Hypromellose	21001141005	1
Caesar & Loretz GmbH...	Methylcellulose	18331806	1
Caesar & Loretz GmbH...	Hypromellose	19069601	1
Caesar & Loretz GmbH...	Hypromellose	20000987004	1
Caesar & Loretz GmbH...	Methylcellulose	20004546004	1
Caesar & Loretz GmbH...	Hypromellose	22001980009	1
Caesar & Loretz GmbH	Methylcellulose	12044922	1
Caesar & Loretz GmbH	Methylcellulose	18045107	1
Caesar & Loretz GmbH	Methylcellulose	18045114	2
Caesar & Loretz GmbH	Hydroxypropylcellulose	18114605	1
Caesar & Loretz GmbH	Hypromellose	18132105	1
Caesar & Loretz GmbH	Hypromellose	18132109	1
Caesar & Loretz GmbH	Hypromellose	18132111	3
Caesar & Loretz GmbH	Methylcellulose	183318022	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Methylcellulose	18331803	4
Caesar & Loretz GmbH	Methylcellulose	18331806	9
Caesar & Loretz GmbH	Hypromellose	19069601	9
Caesar & Loretz GmbH	Hypromellose	19069608	2
Caesar & Loretz GmbH	Hypromellose	19069609	1
Caesar & Loretz GmbH	Methylcellulose	192473003	4
Caesar & Loretz GmbH	Methylcellulose	192473004	7
Caesar & Loretz GmbH	Hypromellose	192852004	1
Caesar & Loretz GmbH	Hypromellose	192852005	7
Caesar & Loretz GmbH	Hydroxypropylcellulose	20000942007	2
Caesar & Loretz GmbH	Hypromellose	20000987003	1
Caesar & Loretz GmbH	Hypromellose	20000987004	2
Caesar & Loretz GmbH	Hypromellose	20000987006	3
Caesar & Loretz GmbH	Hypromellose	20004281002	1
Caesar & Loretz GmbH	Hypromellose	20004281003	6
Caesar & Loretz GmbH	Methylcellulose	20004546004	3
Caesar & Loretz GmbH	Methylcellulose	20004546008	4
Caesar & Loretz GmbH	Methylcellulose	20004546009	2
Caesar & Loretz GmbH	Methylcellulose	20004546013	3
Caesar & Loretz GmbH	Hypromellose	21001141002	7
Caesar & Loretz GmbH	Hypromellose	21001141004	1
Caesar & Loretz GmbH	Hypromellose	21001141005	7
Caesar & Loretz GmbH	Hypromellose	21001141006	8
Caesar & Loretz GmbH	Hypromellose	21001141009	2
Caesar & Loretz GmbH	Methylcellulose	22000891002	4
Caesar & Loretz GmbH	Methylcellulose	22000891011	1
Caesar & Loretz GmbH	Hypromellose	22001980004	2
Caesar & Loretz GmbH	Hypromellose	22001980005	8
Caesar & Loretz GmbH	Hypromellose	22001980009	2
Caesar & Loretz GmbH	Hypromellose	22003524005	2
CAESAR & LORETZ GMBH	Hypromellose	B02-1977101	1
Caesar & Loretz	Hypromellose	17115005	1
Caesar & Loretz	Hypromellose	17115008	1
Caesar & Loretz	Hypromellose	18132116	1
Caesar&Lorenz/AHD	Methylcellulose	18045107	1
Cealo / AHD 19.09.20...	Hypromellose	19069601	1
Cealo/Gehe	Hypromellose	18132101	1
cealo	Methylcellulose	15179602	1
Cealo	Hypromellose	192852004	1
DOW Chemical Company...	Hypromellose	14G02-B11-296850	1
DOW chemical Company...	Hypromellose	15G08-B14-310845	1
Euro OTC	Methylcellulose	10247609	1
Euro OTC	Methylcellulose	15179602	1
Euro OTC	Methylcellulose	16284003	1
Euro OTC	Hypromellose	18132105	1
Euro OTC	Methylcellulose	18331806	1
Euro OTC	Hypromellose	21001141002	1
Fagron	Hypromellose		1
Fagron	Hypromellose	10G09-N03	1
Fagron	Hypromellose	12A30-N02	3
Fagron	Hypromellose	12D03-N03	1
Fagron	Hypromellose	12E02-N03	3
Fagron	Hypromellose	12G23-N03	1
Fagron	Hypromellose	12G23-NO3	1
Fagron	Methylcellulose	12H06-N06	2
Fagron	Hypromellose	12H20-N05	1
Fagron	Methylcellulose	13/26-N04	1
Fagron	Methylcellulose	131301(09)	1
Fagron	Hypromellose	13D03N03	1
Fagron	Hypromellose	13D03-N03	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Methylcellulose	13E02-B03-290531	3
Fagron	Hypromellose	13E02-B03-290532	1
Fagron	Hypromellose	13h09-m04	1
Fagron	Hypromellose	13H09-N04	9
Fagron	Methylcellulose	14A28-B04-295982	1
Fagron	Hypromellose	14C05B03	1
Fagron	Hypromellose	14C05-B03	1
Fagron	Hypromellose	14C-05B03	1
Fagron	Hypromellose	14c05-B03-294708	1
Fagron	Hypromellose	14C05-B03-294708	4
Fagron	Hypromellose	14C05-B03-294711	1
Fagron	Hypromellose	14G02-B11	3
Fagron	Hypromellose	14G02-B11-296850	6
Fagron	Hypromellose	14G02-B11-296851	1
Fagron	Hypromellose	14g02-b11-302118	2
Fagron	Hypromellose	14G02-B11-302118	7
Fagron	Hypromellose	14G02-B11-302119	1
Fagron	Hypromellose	14G02-B11-302121	1
Fagron	Hypromellose	15B02-B05	1
Fagron	Hypromellose	15B02-B05-308852	1
Fagron	Hypromellose	15G08-B14	1
Fagron	Hypromellose	15g08-b14-310845	2
Fagron	Hypromellose	15G08-B14-310845	10
Fagron	Hypromellose	15G08B14314185	2
Fagron	Hypromellose	15g08-b14-314845	1
Fagron	Methylcellulose	15G08B14314845	1
Fagron	Hypromellose	15G08-B14-314845	7
Fagron	Hypromellose	16B16_B07	1
Fagron	Hypromellose	16B16-B07_321327	1
Fagron	Hypromellose	16B16-B07-318276	2
Fagron	Hypromellose	16b16-b07-318531	1
Fagron	Hypromellose	16B16-B07-318531	8
Fagron	Hypromellose	16B16-B07-321327	3
Fagron	Hypromellose	16B-16-B07-321327	1
Fagron	Hypromellose	16B16-B07-321328	1
Fagron	Hypromellose	16B16-B07-321579	1
Fagron	Hypromellose	16B16-B07-323114	3
Fagron	Hypromellose	16B16-B07-325280	7
Fagron	Hypromellose	16H23B-02	1
Fagron	Hypromellose	16H23-B02-325994	1
Fagron	Hypromellose	16H23-B02-332066	8
Fagron	Hypromellose	17115005	1
Fagron	Hypromellose	18A17-B04	2
Fagron	Hypromellose	18A17-B04-345100	5
Fagron	Hypromellose	18A17-B04-346208	1
Fagron	Hypromellose	18D04-B03	4
Fagron	Hypromellose	18D04-B03-348465	6
Fagron	Hypromellose	18D04-B03-350745	3
Fagron	Hypromellose	18D04-B03-35144	1
Fagron	Hypromellose	18D04-B03-352349	1
Fagron	Hypromellose	18D04-B03-352746	4
Fagron	Hypromellose	18D04-B03-355144	3
Fagron	Hypromellose	18G17-B04-194255	1
Fagron	Hypromellose	19G17-B04	5
Fagron	Hypromellose	19G17-B04-194255	5
Fagron	Hypromellose	19G17-B04-194735	3
Fagron	Hypromellose	1A01012N11	1
Fagron	Hypromellose	1J31012N11	3
Fagron	Hypromellose	1K01012N11	1
Fagron	Hypromellose	20110612-2	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Hypromellose	20D22-B02	1
Fagron	Hypromellose	20D22-B02-197710	7
Fagron	Hypromellose	20D22-B02-1977101	1
Fagron	Hypromellose	20D22-B02-197711	4
Fagron	Hypromellose	20D2-B02-197710	1
Fagron	Hypromellose	20G14-B01	3
Fagron	Hypromellose	20G14-B01-201924	1
Fagron	Hypromellose	21B26-B07-218984	1
Fagron	Hypromellose	220401M	1
Fagron	Hypromellose	2818A-01860	1
Fagron	Hypromellose	2H12012N12	1
Fagron	Hypromellose	2Od22-B02-197711	1
Fagron	Hypromellose	2OD22-BO2-197710	1
Fagron	Hypromellose	2x19G17-B04-194735	1
Fagron	Hypromellose	325994	1
Fagron	Hypromellose	349970	1
Fagron	Hypromellose	3G08012N11	1
Fagron	Hypromellose	615I-01860	1
Fagron	Hypromellose	700182-0001	2
Fagron	Hypromellose	9088155	3
Fagron	Hypromellose	B01-2019204	2
Fagron	Hypromellose	B02-1977100	2
Fagron	Hypromellose	B04-1942505	1
Fagron	Hypromellose	B97-2101203	1
Fagron	Hypromellose	D180F8Q011	1
Fagron	Hypromellose	D180HBA012	1
Fagron	Hypromellose	D180J45013	1
Fagron	Hypromellose	YI16012N11	1
Fagron	Hypromellose	ZH19012N12	1
Fargon/Gehe	Hypromellose	18D04-B03-352746	1
Fiebig	Methylcellulose	18045101	1
Fragon/Phoenix	Hypromellose	18D04-b03-349970	1
FRAGON/Poenix	Hypromellose	16B16-B07-18276	1
Gatt-Koller / Phoenix	Hypromellose	14C05-B03-291647	2
Gatt-Koller	Methylcellulose	18045107	1
Gehe / 26.10.12 Fragon	Hypromellose	9D30-N05	1
Gehe amax	Hypromellose	19G17-B04-194735	1
Gehe	Hypromellose	14G02-B11	1
Gehe	Hypromellose	15G08-B14-310845	1
Gehe	Methylcellulose	16284003	1
GEHE	Hypromellose	16H23-B02	1
GEHE	Hypromellose	17115008	1
GEHE	Hypromellose	18049201	1
GEHE	Hypromellose	18A17-B04	3
Gehe	Hypromellose	19069601	1
gehe	Hypromellose	192852004	1
Jenne	Hypromellose	15G08-B14	1
Jenne	Hypromellose	18D04-B03-350745	2
Jenne	Hypromellose	20G14-B01-201924	2
Jenne	Methylcellulose	21B26-B07-213871	1
Kehr	Hypromellose	17115005	1
Klenk	Hypromellose	19069601	2
L12	Hypromellose	16224406	1
L12	Methylcellulose	16284003	1
L12	Hypromellose	17115008	1
L12	Methylcellulose	17170405	1
Nachprüfung 2609	Hypromellose	11H26-N01	1
Nachprüfung	Hypromellose	3082019-3	1
Noweda	Hypromellose	1315505	1
Noweda	Hypromellose	17115008	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Methylcellulose	17170405	1
Noweda	Hydroxypropylcellulose	18114605	1
Noweda	Hypromellose	18132111	1
Noweda	Methylcellulose	18331806	1
Noweda	Hypromellose	18D04-B03-355144	1
Noweda	Hypromellose	19069603	1
Noweda	Hypromellose	2003524007	1
Noweda	Hypromellose	22003524004	2
Noweda	Hypromellose	D180HBA012	1
Phoenix/Cealo	Methylcellulose	17170404	1
Phoenix	Hypromellose	13E02-B03	1
Phoenix	Hypromellose	14c05-b03-294708	1
Phoenix	Hypromellose	16224407	1
Phoenix	Hypromellose	16B16-B07	2
Phoenix	Hypromellose	16B16-B07-321327	1
Phoenix	Methylcellulose	18331803	1
Phoenix	Methylcellulose	23001536003	1
Phönix Gotha	Hypromellose	14G02-B11-296850	1
Phonix	Hypromellose	13H09-N04	1
Phönix	Hypromellose	16224403	1
PHÖNIX	Hypromellose	16H23-B02-325994	1
Phönix	Hypromellose	2000987004	1
Phönix	Hypromellose	23000497003	1
Sanacorp 08.11.21, 22,95EUR	Hypromellose	211125H	1
Sanacorp	Methylcellulose	1717405	1
Sanacorp	Methylcellulose	18331803	1
Sanacorp	Hypromellose	19069608	1
Sanacorp	Hypromellose	22001980005	2
Sanacorp	Hypromellose	23000497003	2
Sanacorp	Hypromellose	2H12012N12	1

- 234 851 spectra from 1515 *Apo-Ident* customers from a total of 48 997 batches from a further 719 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Methylcellulose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Methylcellulose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	1175	0	151 787
Type B	0	770	0	201 314
Type C	0	1202	14	234 851

The substance/substance group *Methylcellulose* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.4894 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2208 %)
Type C	100.0000 % (> 99.9007 %)	98.8487 % (> 98.6020 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20686	20686	0.00	179.52
20705	20705	0.00	155.97
20919	20919	0.00	164.76
20931	20919	7.55	168.38
21570	22457	15.39	157.10
21702	20919	30.72	160.78
21767	21767	0.00	172.56
22258	21767	16.07	177.93
22457	22457	0.00	156.08
22609	26488	17.21	173.94
23224	22457	11.00	156.82
24249	24249	0.00	160.74
25060	26636	32.84	158.18
25188	22457	18.73	152.31
25230	25230	0.00	168.49
25231	25231	0.00	169.51
25286	25286	0.00	151.72
25426	21767	8.30	175.35
25622	25622	0.00	160.91
25981	21767	17.87	171.84
26148	26148	0.00	171.95
26488	26488	0.00	172.66
26636	26636	0.00	153.72
26721	26721	0.00	192.17
27139	27139	0.00	180.80

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Methylprednisolone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20953-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Methylprednisolone; Methylprednisolonum

Special notes

When selecting the *Methylprednisolone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Methylprednisolone	4	4	3

Second-stage model

For differentiation of the substance/substance group *Methylprednisolone* the following second-stage model is used:

- Submodel 02

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Methylprednisolone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	80.06	–
⋮	⋮	⋮
Prednisolone	>50	73.64
Tyrothricin	>50	83.92
Betamethasone	>50	87.57
Triamcinolone acetonide	>50	94.52
Fluocinolone acetonide	>50	97.53
Gramicidin	>50	137.80
Dexamethasone	>50	174.94

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Methylprednisolone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Methylprednisolone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Methylprednisolone	13G19-N05	20953	40	1402438
Fagron	Methylprednisolone	15I04-B05-311572	22275	45	AR-16-FG-009102-01
Fagron	Methylprednisolone	15I04-B05-311572	22275SI	45	AR-16-FG-009102-01
Fagron	Methylprednisolone	15I04-B05-311572	22354	45	20151026
Fagron	Methylprednisolone	15I04-B05-311572	22354SI	45	20151026
Fagron	Methylprednisolone	18E16-B02-B02-358166	24572	40	20180611
Fagron	Methylprednisolone	21C30-F03-377878	25725	50	20210505
Fagron	Methylprednisolone	21C30-F03-377878	25725SI	50	20210505

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 8 reference samples from the substance/substance group *Methylprednisolone*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 152 602 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 310 spectra of 8 reference samples from the substance/substance group *Methylprednisolone*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Methylprednisolone	12D17-N04	20650	40
Fagron	Methylprednisolone	15L15-B01-321887	23229	40
Fagron	Methylprednisolone	18A03-B05-345742	23997	40
Fagron	Methylprednisolone	22D14-B07-227694	26619	40
Fagron	Methylprednisolone	15L15-B01-321887	23229SI	30
Fagron	Methylprednisolone	18A03-B05-345742	23997SI	40
Fagron	Methylprednisolone	18E16-B02-B02-358166	24572SI†	40
Fagron	Methylprednisolone	22D14-B07-227694	26619SI	40

- 201 774 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 3 spectra from 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Methylprednisolone*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Methylprednisolone	22D14-B07-221096	1
Fagron	Methylprednisolone	12D17-N04	1
Fagron	Methylprednisolone	18A03-B05	1

- 236 064 spectra from 1515 *Apo-Ident* customers from a total of 49 255 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Methylprednisolone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Methylprednisolone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	310	0	201 774
Type C	0	3	0	236 064

The substance/substance group *Methylprednisolone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.0645 %)
Type C	100.0000 % (> 99.9011 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20953	20953	0.00	144.55
22275	22275	0.00	149.53
22354	22275	6.08	151.32
24572	22275	12.97	146.98
25725	22275	24.88	143.27

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Metoclopramide hydrochloride monohydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21662-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Metoclopramide hydrochloride monohydrate; Metoclopramidi hydrochloridum monohydricum

Special notes

When selecting the *Metoclopramide hydrochloride monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Metoclopramide hydrochloride monohydrate	6	3	5

Second-stage model

For differentiation of the substance/substance group *Metoclopramide hydrochloride monohydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Metoclopramide hydrochloride monohydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	108.21	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Metoclopramide hydrochloride monohydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Metoclopramide hydrochloride monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Metoclopramide hydrochlor…	14193102	21662	60	AR-15-FG-002889-01
Caelo	Metoclopramide hydrochlor…	14193102	21746	60	20140725
Caelo	Metoclopramide hydrochlor…	15421101	23234	40	20160226
Fagron	Metoclopramide hydrochlor…	20G14-F05-374155	25584	40	20200826
Fagron	Metoclopramide hydrochlor…	22A14-B04-227242	26544	40	20220318
Fagron	Metoclopramide hydrochlor…	23J28-B01-231563	27040	40	20231119
Gatt-Koller	Metoclopramide hydrochlor…	20170236	24410	40	20170724

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 320 spectra of 7 reference samples from the substance/substance group *Metoclopramide hydrochloride monohydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 642 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 6 reference samples from the substance/substance group *Metoclopramide hydrochloride monohydrate*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Metoclopramide hydrochlor…	15421102	23718	40
Fagron	Metoclopramide hydrochlor…	21F07-B08-213763	25863	50
Gatt-Koller	Metoclopramide hydrochlor…	22J02736	26625	40
Fagron	Metoclopramide hydrochlor…	22A14-B04-227242	26544SI†	20
Fagron	Metoclopramide hydrochlor…	23J28-B01-231563	27040SI†	20
Gatt-Koller	Metoclopramide hydrochlor…	22J02736	26625SI	20

- 201 894 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 23 spectra from 22 *Apo-Ident* customers from 5 batches from the substance/substance group *Metoclopramide hydrochloride monohydrate*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Metoclopramide hydrochlor…	14193101	1
Caelo	Metoclopramide hydrochlor…	15227001	18

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metoclopramide hydrochlor…	2818Q-01869	1
Caelo	Metoclopramide hydrochlor…	3414U-018969	1
Caesar&loretz,Phoenix	Metoclopramide hydrochlor…	14193101	1
Fragon/ Sanacorp	Metoclopramide hydrochlor…	1/17M	1

- 236 044 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Metoclopramide hydrochloride monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Metoclopramide hydrochloride monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	190	0	201 894
Type C	0	23	0	236 044

The substance/substance group *Metoclopramide hydrochloride monohydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 73.9130 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21662	21662	0.00	211.03
21746	21662	5.25	211.15
23234	21662	7.78	213.27
24410	21662	6.73	212.75
25584	21662	16.15	214.92
26544	21662	15.12	217.84
27040	21662	16.50	215.37

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Metoprolol tartrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21753-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Metoprolol tartrate; Metoprololi tartras

Special notes

When selecting the *Metoprolol tartrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Metoprolol tartrate	7	3	76

Second-stage model

For differentiation of the substance/substance group *Metoprolol tartrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Metoprolol tartrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	111.72	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Metoprolol tartrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Metoprolol tartrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Metoprolol tartrate	APMTP02218MT	24596	40	20190220
Euro OTC	Metoprolol tartrate	2001021	25098	40	20200116*
Euro OTC	Metoprolol tartrate	2211008	26429	40	20221215*
Euro OTC	Metoprolol tartrate	2211008	26429SI	20	20221215*
Fagron	Metoprolol tartrate	16E31-B03-327107	22927	40	20160627
Fagron	Metoprolol tartrate	16E31-B03-327107	22943	40	20160627
Fagron	Metoprolol tartrate	16E31-B03-327107	22944	40	20160627
Fagron	Metoprolol tartrate	19K20-F03-366934	25061	40	20191218
Inresa	Metoprolol tartrate	3099O5RII	21753	60	AR-15-FG-006635-01
Inresa	Metoprolol tartrate	4050O5RII	21805	60	20140430

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 420 spectra of 10 reference samples from the substance/substance group *Metoprolol tartrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 542 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Metoprolol tartrate*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Metoprolol tartrate	18K26-B01-359370	24825	40
Fagron	Metoprolol tartrate	21E10-F03-378925	25752	40
Inresa	Metoprolol tartrate	405005RIIC	22908	40

- 201 964 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 296 spectra from 192 *Apo-Ident* customers from 82 batches from the substance/substance group *Metoprolol tartrate*.

- Among them are spectra of independent samples from 76 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Metoprolol tartrate		1
	Metoprolol tartrate	2001021-02	4
	Metoprolol tartrate	210530SRII	1
	Metoprolol tartrate	2211008-01	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
	Metoprolol tartrate	22F02-B19-220195	3
AHD	Metoprolol tartrate	22F02-B19-220195	2
Andor	Metoprolol tartrate	APMTP0117MT	1
Antares	Metoprolol tartrate	1014Q-07308	1
apomix	Metoprolol tartrate	18K26-B01-355911	1
Audor Pharma	Metoprolol tartrate	APMTP00117MT	17
Audor Pharma	Metoprolol tartrate	APMTP02218	1
Audor Pharma	Metoprolol tartrate	APMtP02218Mt	1
Audor Pharma	Metoprolol tartrate	APMTP02218MT	16
Audor Pharma	Metoprolol tartrate	APMTPOC117MT	1
Audor Pharma	Metoprolol tartrate	MTP00117MT	1
Audor Pharma	Metoprolol tartrate	MTP02218	1
Caelo	Metoprolol tartrate	1729314P-200715-1	1
Caelo	Metoprolol tartrate	17G03-B09-351672	1
Caelo	Metoprolol tartrate	1919I-03763	1
Caelo	Metoprolol tartrate	APMT00117MT	1
EuRho	Metoprolol tartrate	2001021-02	2
Euro OTC	Metoprolol tartrate	2001021	1
Euro OTC	Metoprolol tartrate	200102101	1
Euro OTC	Metoprolol tartrate	2001021-01	61
Euro OTC	Metoprolol tartrate	2001021-02	8
Euro OTC	Metoprolol tartrate	201021-01	1
Euro OTC	Metoprolol tartrate	AP20112701	1
Euro OTC	Metoprolol tartrate	Meto08122022	1
Euro OTC	Metoprolol tartrate	MTP02218	3
Fagro	Metoprolol tartrate	16MD000095	1
Fagron	Metoprolol tartrate	16E31-B03-325535	1
Fagron	Metoprolol tartrate	16E31-B03-327107	23
Fagron	Metoprolol tartrate	17003O5RII	1
Fagron	Metoprolol tartrate	17G03-B03-353935	1
Fagron	Metoprolol tartrate	17G03-B09	1
Fagron	Metoprolol tartrate	17G03-B09-340197	3
Fagron	Metoprolol tartrate	17G03-B09-342813	2
Fagron	Metoprolol tartrate	17G03-B09-345302	1
Fagron	Metoprolol tartrate	17G03-B09-347089	1
Fagron	Metoprolol tartrate	17G03-B09-347304	1
Fagron	Metoprolol tartrate	17g03-B09-350669	1
Fagron	Metoprolol tartrate	17G03-B09-350669	4
Fagron	Metoprolol tartrate	17G03-B09-351672	1
Fagron	Metoprolol tartrate	17G03-B09-353935	2
Fagron	Metoprolol tartrate	18027O5RII	1
Fagron	Metoprolol tartrate	18K26-B01	2
Fagron	Metoprolol tartrate	18K26-B01-355910	1
Fagron	Metoprolol tartrate	18K26-B01-355911	2
Fagron	Metoprolol tartrate	18K26-B01-359370	7
Fagron	Metoprolol tartrate	18K26-B01-359371	7
Fagron	Metoprolol tartrate	18K26-B01-362451	3
Fagron	Metoprolol tartrate	18KS26-B01	1
Fagron	Metoprolol tartrate	1902205RII	1
Fagron	Metoprolol tartrate	19022O5RII	1
Fagron	Metoprolol tartrate	1902O5RII	1
Fagron	Metoprolol tartrate	19K20-F03	1
Fagron	Metoprolol tartrate	19K20-F03-366934	7
Fagron	Metoprolol tartrate	19K20-F03-366935	1
Fagron	Metoprolol tartrate	19K20-F03-366936	1
Fagron	Metoprolol tartrate	20H06-F04	2
Fagron	Metoprolol tartrate	20H06F04373426	3
Fagron	Metoprolol tartrate	20H06-F04-373426	4
Fagron	Metoprolol tartrate	2100605RII	1
Fagron	Metoprolol tartrate	21E-10-F03	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Metoprolol tartrate	21E10-F03-378925	12
Fagron	Metoprolol tartrate	21E10-F03-378925/2100605RII	1
Fagron	Metoprolol tartrate	21E10-F03378926	1
Fagron	Metoprolol tartrate	21E10-F03-378926	3
Fagron	Metoprolol tartrate	21E10-F03-78926	1
Fagron	Metoprolol tartrate	22F02-B19-220195	1
Fagron	Metoprolol tartrate	22F02-B19-220257	1
Fagron	Metoprolol tartrate	B01-3593700	1
Fagron	Metoprolol tartrate	B01-3624501	1
Fagron	Metoprolol tartrate	F03-3669304	2
Fagron	Metoprolol tartrate	F03-3789205	4
Fagron	Metoprolol tartrate	F04-3734206	1
Fagron	Metoprolol tartrate	FO3-3789205	1
Gehe	Metoprolol tartrate	21E-10-F03	1
Gehe	Metoprolol tartrate	2211008-01	3
Gehe	Metoprolol tartrate	22F02-B19-220195	1
HELIOS Klinikum Erfu…	Metoprolol tartrate	405005RIIC	1
Inresa	Metoprolol tartrate	4050005RIIB	1
Inresa	Metoprolol tartrate	405005RIIB	1
Inresa	Metoprolol tartrate	504005RIIC/29082016	1
Jenne	Metoprolol tartrate	2211008-01	1
Klosterring	Metoprolol tartrate	17G03-B09-345301	1
Noweda 21.06.22 EK 34,95	Metoprolol tartrate	2001021-01	1
Noweda	Metoprolol tartrate	18K26-B01-3593705	1
Noweda	Metoprolol tartrate	18K26-B01-362451	1
Noweda	Metoprolol tartrate	21E10-F03	1
Noweda	Metoprolol tartrate	2211008-01	1
Noweda	Metoprolol tartrate	22F02-B19-220195	1
Noweda	Metoprolol tartrate	F03-3789206	1
Phönix	Metoprolol tartrate	21E10-F03	1
Sanacorp	Metoprolol tartrate	2001021-01	3
Sanacorp	Metoprolol tartrate	2211008-01	3
Sidonia	Metoprolol tartrate	405005RIIC/09062017	1
Sigma Adrich/Alliance H.	Metoprolol tartrate	PHR1076	1
Sigma-Aldrich GmbH	Metoprolol tartrate	LRAA6905	4
Th. Geyer	Metoprolol tartrate	56392-17-7	1

- 235 771 spectra from 1515 *Apo-Ident* customers from a total of 49 177 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Metoprolol tartrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Metoprolol tartrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	120	0	201 964
Type C	0	291	5	235 771

The substance/substance group *Metoprolol tartrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9007 %)	98.3108 % (> 97.2973 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21753	21753	0.00	146.15
21805	21753	5.30	146.75
22927	21753	9.26	141.98
22943	21753	4.68	144.75
22944	25098	7.12	140.54
24596	25098	8.18	141.59
25061	21753	9.40	147.67
25098	25098	0.00	140.54
26429	26429	0.00	142.21

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Metronidazole**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20001-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Metronidazole; Metronidazolum

Special notes

When selecting the *Metronidazole* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Metronidazole	9	26	737

Second-stage model

For differentiation of the substance/substance group *Metronidazole* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Metronidazole* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Menthol	94.13	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Metronidazole* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Metronidazole*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Metronidazole	12110410	20857	40	20120515
Caelo	Metronidazole	13095007	21356	40	20130426
Caelo	Metronidazole	13095007	21360	40	20130426
Caelo	Metronidazole	160892	22472	60	20160413*
Caelo	Metronidazole	20002297	25565	40	20200902*
Euro OTC	Metronidazole	1212030-02	21213	40	20130627
Euro OTC	Metronidazole	1508004	21881	60	20150819*
Euro OTC	Metronidazole	2005029	25330	40	20200820*
Fagron	Metronidazole	13D10-N02	21212	40	20130516
Fagron	Metronidazole	16I19-B04-326155	22835	40	20161013

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 440 spectra of 10 reference samples from the substance/substance group *Metronidazole*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 522 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1130 spectra of 31 reference samples from the substance/substance group *Metronidazole*.

- Among them are spectra of independent samples from 26 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Metronidazole	13095005	21214	40
Caelo	Metronidazole	172905	23808	40
Caelo	Metronidazole	190102	24558	40
Caelo	Metronidazole	21002293	25851	50
Caelo	Metronidazole	22002266	26490	40
Caelo	Metronidazole	23003075	27109	40
Euro OTC	Metronidazole	1609028	22751	40
Euro OTC	Metronidazole	1612013	22917	40
Euro OTC	Metronidazole	1701039	23132	40
Euro OTC	Metronidazole	1707008	23542	30
Euro OTC	Metronidazole	1706022	23550	30
Euro OTC	Metronidazole	1802007	23946	40
Euro OTC	Metronidazole	1807039	24203	40
Euro OTC	Metronidazole	1901042	24449	40
Euro OTC	Metronidazole	1906012	24766	40
Euro OTC	Metronidazole	1908028	24864	40
Euro OTC	Metronidazole	2007002	25328	40
Euro OTC	Metronidazole	2103002	25677	50
Euro OTC	Metronidazole	2207001	26199	40
Euro OTC	Metronidazole	2206031	26204	40
Euro OTC	Metronidazole	2308004	26888	40
Euro OTC	Metronidazole	2308003	26889	40
Euro OTC	Metronidazole	2402031	27145	40
Euro OTC	Metronidazole	2404007	27297	40
Fagron	Metronidazole	17C10-B04-355868	24586	40
Fagron	Metronidazole	21G29-B02-213325	26179	40
Caelo	Metronidazole	21002293	25851SI	10
Caelo	Metronidazole	22002266	26490SI	20
Euro OTC	Metronidazole	2207001	26199SI	20

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Metronidazole	2206031	26204SI	20
Fagron	Metronidazole	21G29-B02-213325	26179SI	20

- 200 954 spectra from a total of 4019 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5455 spectra from 1292 *Apo-Ident* customers from 779 batches from the substance/substance group *Metronidazole*.
- Among them are spectra of independent samples from 733 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Metronidazole		1
	Metronidazole	15253007	2
	Metronidazole	2005029-01	1
	Metronidazole	2007002-02	4
	Metronidazole	21002293005	1
	Metronidazole	21002293011	2
	Metronidazole	21002293016	4
	Metronidazole	21002293020	22
	Metronidazole	2103002-01	1
	Metronidazole	2103002-03	1
	Metronidazole	2103002-1	1
	Metronidazole	21G29-B02-213325	1
	Metronidazole	21G29-B02-221739	2
	Metronidazole	22002266002	4
	Metronidazole	22002266003	3
	Metronidazole	22002266004	7
	Metronidazole	22002266005	1
	Metronidazole	22002266006	9
	Metronidazole	22002266007	6
	Metronidazole	22002266008	24
	Metronidazole	22002266009	6
	Metronidazole	22002266010	20
	Metronidazole	2200226608	1
	Metronidazole	2202266003	1
	Metronidazole	2206031-01	3
	Metronidazole	2206031-02	1
	Metronidazole	2207001-01	4
	Metronidazole	230800-01	1
	Metronidazole	2308003-01	5
	Metronidazole	2308004-01	3
	Metronidazole	2308004-02	1
	Metronidazole	24000389002	4
	Metronidazole	24000389003	2
	Metronidazole	24000389006	1
17270001	Metronidazole	17058026	1
A.H. 19.02.13 ek: 5,86EUR	Metronidazole	12G04-N15	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
ACM	Metronidazole		1
AEP	Metronidazole	22002266008	1
Aep	Metronidazole	2202266008	1
AHD 03.02.17	Metronidazole	16089212	1
AHD 13.10.17 E.k:6,56	Metronidazole	17058003	1
AHD	Metronidazole	13214025	1
AHD	Metronidazole	15253005	1
AHD	Metronidazole	15253033	1
AHD	Metronidazole	16I19-B04-329160	2
AHD	Metronidazole	17290518	1
AHD	Metronidazole	19000516007	1
AHD	Metronidazole	21002293005	1
AHD	Metronidazole	21002293006	1
AHD	Metronidazole	21002293019	1
AHD	Metronidazole	22002266003	1
AHD	Metronidazole	22002266004	1
AHD	Metronidazole	220022660058	1
AHD	Metronidazole	22002266008	3
ALH	Metronidazole	1609028-01	1
Alliance Health 20.0...	Metronidazole	1307042-01	2
Alliance Health 23.0...	Metronidazole	1212001-02	1
Alliance Healthcare	Metronidazole	12110415	1
Alliance Healthcare	Metronidazole	20004568008	1
Alliance	Metronidazole	12339502	1
Alliance	Metronidazole	22002266008	1
alliance	Metronidazole	2206031-01	1
Allianz Healthcare	Metronidazole	19g02-b04	1
Anzag 21.10.14 EK 2.85	Metronidazole	13095007	1
Anzag 15.12.17 3.41	Metronidazole	1705812	1
Anzag	Metronidazole	11373512	1
anzag	Metronidazole	14C14-B02-291276	2
Anzag	Metronidazole	1505024-01	1
Anzag	Metronidazole	15253022	1
Anzag	Metronidazole	20004568005	1
Anzag;14,21EUR;16.04.15	Metronidazole	13214012	1
api-ident	Metronidazole	16/19-B04	1
Apo Ident	Metronidazole	1807039-03	1
Apoident,Phönix, 09....	Metronidazole	1701039-01	1
Apo-ident	Metronidazole	108703902	1
apo-ident	Metronidazole	1807039-01	2
apo-ident	Metronidazole	1901042-01	2
Apotheke an der Born...	Metronidazole	16089223	1
Audor Pharma	Metronidazole	1908028-02	1
Audor Pharma	Metronidazole	2007002-01	1
Bombastus	Metronidazole	123Validierung	1
Bombastus	Metronidazole	13214018	1
Bombastus	Metronidazole	15253032	1
Bombastus	Metronidazole	16089220	1
Bombastus	Metronidazole	1609028-01	1
Bombastus	Metronidazole	17C10-B04-346280	1
Bombastus	Metronidazole	18026401	1
Caelo	Metronidazole		7
Caelo	Metronidazole	10112903	1
Caelo	Metronidazole	10112907	1
Caelo	Metronidazole	102311870	1
Caelo	Metronidazole	10368310	1
Caelo	Metronidazole	10368311	1
Caelo	Metronidazole	10368313	1
Caelo	Metronidazole	10368318	1
Caelo	Metronidazole	10368319	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metronidazole	1061804	2
Caelo	Metronidazole	1109030-01	2
Caelo	Metronidazole	1112028-01	1
Caelo	Metronidazole	11319807	1
Caelo	Metronidazole	11319810	2
Caelo	Metronidazole	11319812	1
Caelo	Metronidazole	11319816	2
Caelo	Metronidazole	11319818	2
Caelo	Metronidazole	11319819	1
Caelo	Metronidazole	11319823	5
Caelo	Metronidazole	11319824	2
Caelo	Metronidazole	11319825	3
Caelo	Metronidazole	113214021	1
Caelo	Metronidazole	11F15-N07	1
Caelo	Metronidazole	11h11-n03	1
Caelo	Metronidazole	1201156	1
Caelo	Metronidazole	12081507	1
Caelo	Metronidazole	12091403	1
Caelo	Metronidazole	1210411	1
Caelo	Metronidazole	12110105	1
Caelo	Metronidazole	12110403	1
Caelo	Metronidazole	12110405	8
Caelo	Metronidazole	121104085	1
Caelo	Metronidazole	12110411	5
Caelo	Metronidazole	12110412	5
Caelo	Metronidazole	12110413	4
Caelo	Metronidazole	12110414	3
Caelo	Metronidazole	12110415	4
Caelo	Metronidazole	12110421	6
Caelo	Metronidazole	12110422	16
Caelo	Metronidazole	12110423	1
Caelo	Metronidazole	121203001	2
Caelo	Metronidazole	1212030-21	1
Caelo	Metronidazole	12339501	7
Caelo	Metronidazole	12339502	18
Caelo	Metronidazole	12339503	6
Caelo	Metronidazole	12339504	6
Caelo	Metronidazole	12339507	7
Caelo	Metronidazole	12339508	4
Caelo	Metronidazole	12339509	4
Caelo	Metronidazole	12339510	10
Caelo	Metronidazole	12339511	14
Caelo	Metronidazole	12339519	12
Caelo	Metronidazole	12339520	4
Caelo	Metronidazole	12339521	1
Caelo	Metronidazole	12339526	1
Caelo	Metronidazole	12359501	1
Caelo	Metronidazole	1239504	1
Caelo	Metronidazole	12L17-N11	3
Caelo	Metronidazole	13041503	1
Caelo	Metronidazole	1307002	1
Caelo	Metronidazole	1307002-02	1
Caelo	Metronidazole	1307042-01	1
Caelo	Metronidazole	13095001	10
Caelo	Metronidazole	13095002	8
Caelo	Metronidazole	13095003	11
Caelo	Metronidazole	13095004	12
Caelo	Metronidazole	13095005	4
Caelo	Metronidazole	13095006	7
Caelo	Metronidazole	13095007	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metronidazole	13095011	3
Caelo	Metronidazole	13095012	13
Caelo	Metronidazole	13095013	13
Caelo	Metronidazole	13095017	3
Caelo	Metronidazole	13095018	6
Caelo	Metronidazole	13095019	7
Caelo	Metronidazole	13095020	5
Caelo	Metronidazole	1314013	1
Caelo	Metronidazole	13214001	13
Caelo	Metronidazole	13214002	17
Caelo	Metronidazole	132140022	1
Caelo	Metronidazole	13214003	11
Caelo	Metronidazole	13214009	7
Caelo	Metronidazole	13214010	5
Caelo	Metronidazole	13214011	2
Caelo	Metronidazole	13214012	3
Caelo	Metronidazole	13214013	1
Caelo	Metronidazole	13214014	10
Caelo	Metronidazole	13214015	8
Caelo	Metronidazole	13214016	3
Caelo	Metronidazole	13214017	3
Caelo	Metronidazole	13214018	4
Caelo	Metronidazole	13214019	9
Caelo	Metronidazole	13214021	1
Caelo	Metronidazole	13214024	4
Caelo	Metronidazole	13214025	6
Caelo	Metronidazole	13214029	9
Caelo	Metronidazole	1321409	1
Caelo	Metronidazole	13J21-N07	1
Caelo	Metronidazole	1407003-01	1
Caelo	Metronidazole	1407003-2	1
Caelo	Metronidazole	14111304	1
Caelo	Metronidazole	1412016-01	4
Caelo	Metronidazole	1412016-02	1
Caelo	Metronidazole	14b27-b31-291230	1
Caelo	Metronidazole	14B27-B31-291230	1
Caelo	Metronidazole	14B27-B31-291234	1
Caelo	Metronidazole	14c14-b01-295545	1
Caelo	Metronidazole	14C14-B02-291237	1
Caelo	Metronidazole	14C14-B02-291239	1
Caelo	Metronidazole	14C14-B02-291276	1
Caelo	Metronidazole	1505024-02	2
Caelo	Metronidazole	1508004-01	2
Caelo	Metronidazole	1508004-02	1
Caelo	Metronidazole	15121202	1
Caelo	Metronidazole	15215103	4
Caelo	Metronidazole	15215104	5
Caelo	Metronidazole	15215105	1
Caelo	Metronidazole	15215106	5
Caelo	Metronidazole	15215107	1
Caelo	Metronidazole	15215108	10
Caelo	Metronidazole	1523006	1
Caelo	Metronidazole	1523013	1
Caelo	Metronidazole	1523017	1
Caelo	Metronidazole	1523026	1
Caelo	Metronidazole	1525016	1
Caelo	Metronidazole	15253001	13
Caelo	Metronidazole	15253002	5
Caelo	Metronidazole	15253003	9
Caelo	Metronidazole	15253004	14

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metronidazole	15253005	3
Caelo	Metronidazole	15253006	10
Caelo	Metronidazole	15253007	13
Caelo	Metronidazole	15253011	11
Caelo	Metronidazole	15253013	12
Caelo	Metronidazole	15253013/2016030911	1
Caelo	Metronidazole	15253015	15
Caelo	Metronidazole	15253016	13
Caelo	Metronidazole	15253017	14
Caelo	Metronidazole	15253018	6
Caelo	Metronidazole	15253019	3
Caelo	Metronidazole	15253020	5
Caelo	Metronidazole	15253021	9
Caelo	Metronidazole	15253022	7
Caelo	Metronidazole	15253024	12
Caelo	Metronidazole	15253026	19
Caelo	Metronidazole	15253027	13
Caelo	Metronidazole	15253028	9
Caelo	Metronidazole	15253029	5
Caelo	Metronidazole	15253032	13
Caelo	Metronidazole	15253033	7
Caelo	Metronidazole	15253034	1
Caelo	Metronidazole	15258016	1
Caelo	Metronidazole	15A20-B07-303293	1
Caelo	Metronidazole	15A20-B07-303297	1
Caelo	Metronidazole	15A20-B07-303298	1
Caelo	Metronidazole	16/19-B04-326150	1
Caelo	Metronidazole	16/19-B04-326155	1
Caelo	Metronidazole	16/19-B04-329160	1
Caelo	Metronidazole	16051703	1
Caelo	Metronidazole	16056235	1
Caelo	Metronidazole	16089123	1
Caelo	Metronidazole	1608918	1
Caelo	Metronidazole	16089201	7
Caelo	Metronidazole	16089202	11
Caelo	Metronidazole	16089209	16
Caelo	Metronidazole	16089212	19
Caelo	Metronidazole	16089213	21
Caelo	Metronidazole	16089215	14
Caelo	Metronidazole	16089215/1140217	1
Caelo	Metronidazole	16089216	8
Caelo	Metronidazole	16089217	9
Caelo	Metronidazole	16089218	13
Caelo	Metronidazole	16089219	17
Caelo	Metronidazole	16089220	19
Caelo	Metronidazole	16089221	12
Caelo	Metronidazole	16089222	11
Caelo	Metronidazole	16089223	5
Caelo	Metronidazole	16089224	5
Caelo	Metronidazole	16089225	1
Caelo	Metronidazole	16089228	14
Caelo	Metronidazole	16089228-20170818Ma4	1
Caelo	Metronidazole	16089229	13
Caelo	Metronidazole	16089231	4
Caelo	Metronidazole	16089235	11
Caelo	Metronidazole	16089236	3
Caelo	Metronidazole	160892365302	1
Caelo	Metronidazole	160902801	1
Caelo	Metronidazole	1609028-01	7
Caelo	Metronidazole	161201301	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metronidazole	1612013-01	1
Caelo	Metronidazole	1619-b04-326150	1
Caelo	Metronidazole	16253015	1
Caelo	Metronidazole	16D15-B50-324137	1
Caelo	Metronidazole	16I19-B04-329167	1
Caelo	Metronidazole	1701039-01	2
Caelo	Metronidazole	170580001	2
Caelo	Metronidazole	17058001	14
Caelo	Metronidazole	17058002	11
Caelo	Metronidazole	17058003	14
Caelo	Metronidazole	170580035444	1
Caelo	Metronidazole	17058004	9
Caelo	Metronidazole	17058005	14
Caelo	Metronidazole	1705801	1
Caelo	Metronidazole	17058010	14
Caelo	Metronidazole	17058011	18
Caelo	Metronidazole	17058012	21
Caelo	Metronidazole	17058012/2231117	1
Caelo	Metronidazole	170580123	1
Caelo	Metronidazole	17058013	17
Caelo	Metronidazole	17058013-20180404Ma4	1
Caelo	Metronidazole	17058013-20180619Ma6	1
Caelo	Metronidazole	17058014	20
Caelo	Metronidazole	17058015	19
Caelo	Metronidazole	17058016	27
Caelo	Metronidazole	170580165554	1
Caelo	Metronidazole	17058017	16
Caelo	Metronidazole	17058018	24
Caelo	Metronidazole	17058019	22
Caelo	Metronidazole	17058026	19
Caelo	Metronidazole	17058027	15
Caelo	Metronidazole	1706022-01	2
Caelo	Metronidazole	17070008-01	1
Caelo	Metronidazole	1707008-01	6
Caelo	Metronidazole	1707008-02	1
Caelo	Metronidazole	17250517	1
Caelo	Metronidazole	1729027	1
Caelo	Metronidazole	17290503	25
Caelo	Metronidazole	17290504	24
Caelo	Metronidazole	17290506	27
Caelo	Metronidazole	17290507	26
Caelo	Metronidazole	17290509	10
Caelo	Metronidazole	17290512	30
Caelo	Metronidazole	172905125723	1
Caelo	Metronidazole	17290513	5
Caelo	Metronidazole	17290515	3
Caelo	Metronidazole	17290517	51
Caelo	Metronidazole	17290518	58
Caelo	Metronidazole	17290519	10
Caelo	Metronidazole	17290525	52
Caelo	Metronidazole	17290526	15
Caelo	Metronidazole	17290527	49
Caelo	Metronidazole	17290532	34
Caelo	Metronidazole	17290533	31
Caelo	Metronidazole	17290534	3
Caelo	Metronidazole	17290625	1
Caelo	Metronidazole	172990507	1
Caelo	Metronidazole	174058019	1
Caelo	Metronidazole	175058013	1
Caelo	Metronidazole	1758017	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metronidazole	1790504	1
Caelo	Metronidazole	1790512	1
Caelo	Metronidazole	1790517	1
Caelo	Metronidazole	179290525	1
Caelo	Metronidazole	17C10-B04-346275	2
Caelo	Metronidazole	17C10-B04-346280	1
Caelo	Metronidazole	1802007-01	1
Caelo	Metronidazole	180264001	1
Caelo	Metronidazole	18026401	14
Caelo	Metronidazole	18051201	1
Caelo	Metronidazole	18061803	1
Caelo	Metronidazole	1807039-01	2
Caelo	Metronidazole	1807039-03	1
Caelo	Metronidazole	18071401	1
Caelo	Metronidazole	18B28-B50	1
Caelo	Metronidazole	190000516008	1
Caelo	Metronidazole	1900016019	1
Caelo	Metronidazole	19000512012	1
Caelo	Metronidazole	190005160	1
Caelo	Metronidazole	19000516001	16
Caelo	Metronidazole	190005160016	1
Caelo	Metronidazole	19000516002	44
Caelo	Metronidazole	19000516003	8
Caelo	Metronidazole	19000516006	35
Caelo	Metronidazole	19000516007	34
Caelo	Metronidazole	19000516008	27
Caelo	Metronidazole	19000516010	40
Caelo	Metronidazole	190005-16010	1
Caelo	Metronidazole	19000516012	12
Caelo	Metronidazole	19000516016	33
Caelo	Metronidazole	19000516017	18
Caelo	Metronidazole	19000516019	19
Caelo	Metronidazole	1900214	1
Caelo	Metronidazole	1900516010	2
Caelo	Metronidazole	1901020	1
Caelo	Metronidazole	190102003	4
Caelo	Metronidazole	19010201	25
Caelo	Metronidazole	19010202	25
Caelo	Metronidazole	19010203	35
Caelo	Metronidazole	19010210	23
Caelo	Metronidazole	19010211	35
Caelo	Metronidazole	19010212	37
Caelo	Metronidazole	19010213	23
Caelo	Metronidazole	19010214	19
Caelo	Metronidazole	19010215	24
Caelo	Metronidazole	19010216	20
Caelo	Metronidazole	19011909	1
Caelo	Metronidazole	19012011	1
Caelo	Metronidazole	1901210	1
Caelo	Metronidazole	1901214	1
Caelo	Metronidazole	190601201	1
Caelo	Metronidazole	190802802	1
Caelo	Metronidazole	1910203	1
Caelo	Metronidazole	1957059	1
Caelo	Metronidazole	1957069	1
Caelo	Metronidazole	19G02-B04-362815	1
Caelo	Metronidazole	200004568003	1
Caelo	Metronidazole	200004568004	1
Caelo	Metronidazole	200004568005	1
Caelo	Metronidazole	200004568008	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metronidazole	20001568016	1
Caelo	Metronidazole	20004567001	8
Caelo	Metronidazole	20004568001	2
Caelo	Metronidazole	200045680013	1
Caelo	Metronidazole	200045680016	1
Caelo	Metronidazole	20004568003	46
Caelo	Metronidazole	20004568004	30
Caelo	Metronidazole	20004568005	39
Caelo	Metronidazole	20004568008	9
Caelo	Metronidazole	20004568009	50
Caelo	Metronidazole	20004568012	2
Caelo	Metronidazole	20004568013	19
Caelo	Metronidazole	20004568015	18
Caelo	Metronidazole	20004568016	15
Caelo	Metronidazole	2000456809	1
Caelo	Metronidazole	2004568009	1
Caelo	Metronidazole	2004568016	1
Caelo	Metronidazole	200700201	1
Caelo	Metronidazole	200702-01	1
Caelo	Metronidazole	20121121	1
Caelo	Metronidazole	2013U-01870	1
Caelo	Metronidazole	20140612-12	1
Caelo	Metronidazole	2022015B	1
Caelo	Metronidazole	2071304	1
Caelo	Metronidazole	20G07f03372286	1
Caelo	Metronidazole	210002293014	1
Caelo	Metronidazole	210004568015	1
Caelo	Metronidazole	21002293002	5
Caelo	Metronidazole	21002293003	21
Caelo	Metronidazole	21002293004	6
Caelo	Metronidazole	21002293005	15
Caelo	Metronidazole	21002293006	22
Caelo	Metronidazole	21002293007	1
Caelo	Metronidazole	21002293009	10
Caelo	Metronidazole	21002293010	7
Caelo	Metronidazole	21002293011	12
Caelo	Metronidazole	21002293014	14
Caelo	Metronidazole	21002293016	9
Caelo	Metronidazole	21002293017	5
Caelo	Metronidazole	21002293019	3
Caelo	Metronidazole	21002293020	1
Caelo	Metronidazole	2100293005	1
Caelo	Metronidazole	220022656003	1
Caelo	Metronidazole	22002266003	5
Caelo	Metronidazole	22002266004	1
Caelo	Metronidazole	22002266006	5
Caelo	Metronidazole	2200226608	1
Caelo	Metronidazole	2202266003	1
Caelo	Metronidazole	220226606	1
Caelo	Metronidazole	22040734	1
Caelo	Metronidazole	23011504	1
Caelo	Metronidazole	23021713	1
Caelo	Metronidazole	2619A-01870	1
Caelo	Metronidazole	27092014A	1
Caelo	Metronidazole	2750	1
Caelo	Metronidazole	280218010	1
Caelo	Metronidazole	28061204	1
Caelo	Metronidazole	2813E1870	1
Caelo	Metronidazole	3112M-01870	1
Caelo	Metronidazole	320F01870	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Metronidazole	3301	1
Caelo	Metronidazole	338(intern)	1
Caelo	Metronidazole	39/AKD16	1
Caelo	Metronidazole	39/AKD4	1
Caelo	Metronidazole	3947/V04/16	1
Caelo	Metronidazole	473800045689	1
Caelo	Metronidazole	49(17290526)	1
Caelo	Metronidazole	51(19000516012)	1
Caelo	Metronidazole	6003	1
Caelo	Metronidazole	604081626	1
Caelo	Metronidazole	607211870	1
Caelo	Metronidazole	614U1870	1
Caelo	Metronidazole	7031401	1
Caelo	Metronidazole	7071405	1
Caelo	Metronidazole	7091714	1
Caelo	Metronidazole	8012014B	1
Caelo	Metronidazole	820I-01870	1
Caelo	Metronidazole	9715621	1
Caelo	Metronidazole	C04171127	1
Caelo	Metronidazole	ch17290513	1
Caelo	Metronidazole	F170013	1
Caelo	Metronidazole	I-13095005	1
Caelo	Metronidazole	MZ3847368	1
Caeolo/Phönix	Metronidazole	16089228	1
Caeolo/Sanacorp	Metronidazole	17058019	1
Caeolo/Sanacorp	Metronidazole	17290518	1
Caesar & Lorenz GmbH	Metronidazole	15253013	1
Caesar & Lorenz/Hold...	Metronidazole	20004568013	2
Caesar & Lorenz	Metronidazole	13095013	1
Caesar & Loretz / AHD	Metronidazole	19000516008	1
Caesar & Loretz / AHD	Metronidazole	19010210	2
Caesar & Loretz /Phönix	Metronidazole	19000516007	1
Caesar & Loretz GmbH...	Metronidazole	17058001	1
Caesar & Loretz GmbH...	Metronidazole	17290532	1
Caesar & Loretz GmbH...	Metronidazole	19000516007	1
Caesar & Loretz GmbH...	Metronidazole	19000516017	1
Caesar & Loretz GmbH...	Metronidazole	19010215	1
Caesar & Loretz GmbH...	Metronidazole	20004568009	1
Caesar & Loretz GmbH...	Metronidazole	20004568016	2
Caesar & Loretz GmbH...	Metronidazole	21002293019	1
Caesar & Loretz GmbH...	Metronidazole	22002266003	1
Caesar & Loretz GmbH...	Metronidazole	19000516006	1
Caesar & Loretz GmbH...	Metronidazole	20004568016	1
Caesar & Loretz GmbH...	Metronidazole	19010212	1
Caesar & Loretz GmbH...	Metronidazole	19010213	1
Caesar & Loretz GmbH...	Metronidazole	19000516016	1
Caesar & Loretz GmbH...	Metronidazole	21002293010	1
Caesar & Loretz GmbH...	Metronidazole	19010214	1
Caesar & Loretz GmbH...	Metronidazole	19000516016	1
Caesar & Loretz GmbH...	Metronidazole	21002293003	1
Caesar & Loretz GmbH...	Metronidazole	19000516006	1
Caesar & Loretz GmbH...	Metronidazole	19010211	1
Caesar & Loretz GmbH...	Metronidazole	19000516002	1
Caesar & Loretz GmbH...	Metronidazole	19000516019	1
Caesar & Loretz GmbH...	Metronidazole	19010214	1
Caesar & Loretz GmbH...	Metronidazole	21002293006	1
Caesar & Loretz GmbH...	Metronidazole	17290525	1
Caesar & Loretz GmbH...	Metronidazole	21002293006	1
Caesar & Loretz GmbH...	Metronidazole	21002293010	1
Caesar & Loretz GmbH...	Metronidazole	19000516002	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Metronidazole	19010203	1
Caesar & Loretz GmbH...	Metronidazole	20004568003	1
Caesar & Loretz GmbH/AHD	Metronidazole	19000516006	1
Caesar & Loretz GmbH/AHD	Metronidazole	20004568013	1
Caesar & Loretz GmbH/AHD	Metronidazole	21002293002	1
Caesar & Loretz GmbH/AHD	Metronidazole	21002293011	1
Caesar & Loretz GmbH...	Metronidazole	20004568004	2
Caesar & Loretz GmbH...	Metronidazole	19000516002	1
Caesar & Loretz GmbH...	Metronidazole	19000516019	1
Caesar & Loretz GmbH...	Metronidazole	20004568009	1
Caesar & Loretz GmbH...	Metronidazole	21002293009	1
Caesar & Loretz GmbH/G	Metronidazole	19010211	1
Caesar & Loretz GmbH/G	Metronidazole	20004568009	1
Caesar & Loretz GmbH/Gehe	Metronidazole	19000516001	1
Caesar & Loretz GmbH/Gehe	Metronidazole	19000516007	1
Caesar & Loretz GmbH/gehe	Metronidazole	19000516008	2
Caesar & Loretz GmbH/Gehe	Metronidazole	19010201	2
Caesar & Loretz GmbH/gehe	Metronidazole	19010202	1
Caesar & Loretz GmbH/Gehe	Metronidazole	1908028-01	1
Caesar & Loretz GmbH/Gehe	Metronidazole	20004568005	1
Caesar & Loretz GmbH/GEHE	Metronidazole	20004568016	1
Caesar & Loretz GmbH/Gehe	Metronidazole	21002293005	1
Caesar & Loretz GmbH...	Metronidazole	19000516003	1
Caesar & Loretz GmbH...	Metronidazole	21002293010	2
Caesar & Loretz GmbH...	Metronidazole	19010214	1
Caesar & Loretz GmbH...	Metronidazole	21002293003	1
Caesar & Loretz GmbH...	Metronidazole	19000516002	1
Caesar & Loretz GmbH...	Metronidazole	20004568003	2
Caesar & Loretz GmbH...	Metronidazole	21002293003	3
Caesar & Loretz GmbH...	Metronidazole	1807039-02	1
Caesar & Loretz GmbH...	Metronidazole	190102003	1
Caesar & Loretz GmbH...	Metronidazole	19010212	1
Caesar & Loretz GmbH...	Metronidazole	19010213	1
Caesar & Loretz GmbH...	Metronidazole	20004567001	1
Caesar & Loretz GmbH...	Metronidazole	20004568005	1
Caesar & Loretz GmbH...	Metronidazole	21002293004	1
Caesar & Loretz GmbH/K	Metronidazole	20004568005	1
Caesar & Loretz GmbH/Kehr	Metronidazole	19000516016	1
Caesar & Loretz GmbH...	Metronidazole	19000516007	1
Caesar & Loretz GmbH...	Metronidazole	20004568003	1
Caesar & Loretz GmbH...	Metronidazole	20004568005	1
Caesar & Loretz GmbH...	Metronidazole	19000516002	1
Caesar & Loretz GmbH...	Metronidazole	19000516010	5
Caesar & Loretz GmbH...	Metronidazole	19010203	2
Caesar & Loretz GmbH...	Metronidazole	21002293009	1
Caesar & Loretz GmbH/Ph	Metronidazole	19010212	2
Caesar & Loretz GmbH/PHoe	Metronidazole	19000516010	1
Caesar & Loretz GmbH...	Metronidazole	19000516007	1
Caesar & Loretz GmbH...	Metronidazole	19010210	1
Caesar & Loretz GmbH...	Metronidazole	17290527	1
Caesar & Loretz GmbH...	Metronidazole	19010215	1
Caesar & Loretz GmbH...	Metronidazole	20004568003	1
Caesar & Loretz GmbH...	Metronidazole	20004568009	1
Caesar & Loretz GmbH...	Metronidazole	20004568013	2
Caesar & Loretz GmbH...	Metronidazole	20004568016	1
Caesar & Loretz GmbH...	Metronidazole	22002266008	1
Caesar & Loretz GmbH...	Metronidazole	19000516010	1
Caesar & Loretz GmbH...	Metronidazole	19000516012	1
Caesar & Loretz GmbH...	Metronidazole	19000516017	2
Caesar & Loretz GmbH...	Metronidazole	19010213	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Metronidazole	20004568004	2
Caesar & Loretz GmbH...	Metronidazole	20004568009	2
Caesar & Loretz GmbH...	Metronidazole	21002293004	1
Caesar & Loretz GmbH...	Metronidazole	21002293009	1
Caesar & Loretz GmbH...	Metronidazole	21002293010	1
Caesar & Loretz GmbH...	Metronidazole	22002266003	1
Caesar & Loretz GmbH...	Metronidazole	AP220630-01	1
Caesar & Loretz GmbH	Metronidazole	15253017	1
Caesar & Loretz GmbH	Metronidazole	16089224	1
Caesar & Loretz GmbH	Metronidazole	17058027	1
Caesar & Loretz GmbH	Metronidazole	17290504	3
Caesar & Loretz GmbH	Metronidazole	17290512	1
Caesar & Loretz GmbH	Metronidazole	17290517	6
Caesar & Loretz GmbH	Metronidazole	17290518	2
Caesar & Loretz GmbH	Metronidazole	17290525	10
Caesar & Loretz GmbH	Metronidazole	17290526	7
Caesar & Loretz GmbH	Metronidazole	17290527	7
Caesar & Loretz GmbH	Metronidazole	17290532	2
Caesar & Loretz GmbH	Metronidazole	17290533	4
Caesar & Loretz GmbH	Metronidazole	17290534	2
Caesar & Loretz GmbH	Metronidazole	19000516001	4
Caesar & Loretz GmbH	Metronidazole	19000516002	12
Caesar & Loretz GmbH	Metronidazole	19000516006	11
Caesar & Loretz GmbH	Metronidazole	19000516007	8
Caesar & Loretz GmbH	Metronidazole	19000516008	13
Caesar & Loretz GmbH	Metronidazole	19000516010	14
Caesar & Loretz GmbH	Metronidazole	19000516012	11
Caesar & Loretz GmbH	Metronidazole	19000516016	9
Caesar & Loretz GmbH	Metronidazole	19000516017	10
Caesar & Loretz GmbH	Metronidazole	19000516019	4
Caesar & Loretz GmbH	Metronidazole	190102002	1
Caesar & Loretz GmbH	Metronidazole	190102003	2
Caesar & Loretz GmbH	Metronidazole	19010201	4
Caesar & Loretz GmbH	Metronidazole	19010202	10
Caesar & Loretz GmbH	Metronidazole	19010203	12
Caesar & Loretz GmbH	Metronidazole	19010210	5
Caesar & Loretz GmbH	Metronidazole	19010211	15
Caesar & Loretz GmbH	Metronidazole	19010212	6
Caesar & Loretz GmbH	Metronidazole	19010213	8
Caesar & Loretz GmbH	Metronidazole	19010214	4
Caesar & Loretz GmbH	Metronidazole	19010215	1
Caesar & Loretz GmbH	Metronidazole	19010216	5
Caesar & Loretz GmbH	Metronidazole	19G02	1
Caesar & Loretz GmbH	Metronidazole	19G02-B04	1
Caesar & Loretz GmbH	Metronidazole	20004567001	2
Caesar & Loretz GmbH	Metronidazole	20004568003	13
Caesar & Loretz GmbH	Metronidazole	20004568004	19
Caesar & Loretz GmbH	Metronidazole	20004568005	25
Caesar & Loretz GmbH	Metronidazole	20004568008	7
Caesar & Loretz GmbH	Metronidazole	20004568009	17
Caesar & Loretz GmbH	Metronidazole	20004568013	5
Caesar & Loretz GmbH	Metronidazole	20004568015	1
Caesar & Loretz GmbH	Metronidazole	20004568016	13
Caesar & Loretz GmbH	Metronidazole	21002293002	2
Caesar & Loretz GmbH	Metronidazole	21002293003	6
Caesar & Loretz GmbH	Metronidazole	21002293004	6
Caesar & Loretz GmbH	Metronidazole	21002293005	7
Caesar & Loretz GmbH	Metronidazole	21002293006	8
Caesar & Loretz GmbH	Metronidazole	21002293007	1
Caesar & Loretz GmbH	Metronidazole	21002293009	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Metronidazole	21002293010	6
Caesar & Loretz GmbH	Metronidazole	21002293011	4
Caesar & Loretz GmbH	Metronidazole	21002293014	7
Caesar & Loretz GmbH	Metronidazole	21002293017	7
Caesar & Loretz GmbH	Metronidazole	21002293019	3
Caesar & Loretz GmbH	Metronidazole	21002293020	1
Caesar & Loretz GmbH	Metronidazole	22002266003	3
Caesar & Loretz GmbH	Metronidazole	22002266006	2
Caesar & Loretz GmbH	Metronidazole	22002266007	2
Caesar & Loretz GmbH	Metronidazole	22002266008	1
Caesar & Loretz GmbH	Metronidazole	9000516006	1
Caesar & Loretz GmbH...	Metronidazole	19010202	1
Caesar & Loretz GmbH...	Metronidazole	19G02-B04-362816	1
Caesar & Loretz Hilden	Metronidazole	17290518	1
Caesar & Loretz Hilden	Metronidazole	19000516008	1
Caesar & Loretz Hilden	Metronidazole	19010212	1
Caesar & Loretz Hilden	Metronidazole	19010214	1
Caesar & Loretz/AHD	Metronidazole	19000516010	1
Caesar & Loretz/Geil...	Metronidazole	17290525	1
Caesar & Loretz/Geil...	Metronidazole	19000516008	1
Caesar & Loretz/Geil...	Metronidazole	19010211	1
Caesar & Loretz/Noweda	Metronidazole	20004568009	1
Caesar & Loretz	Metronidazole	16089212	1
Caesar & Loretz	Metronidazole	17058003	1
Caesar & Loretz	Metronidazole	17058019	1
Caesar & Loretz	Metronidazole	17290512	1
Caesar Loretz	Metronidazole	19000516006	1
Caesar u. Loretz GmbH	Metronidazole	19000516008	1
Caesar u. Loretz GmbH	Metronidazole	19000516016	1
Caesar u. Loretz GmbH	Metronidazole	20004568009	1
Caesar und Loretz GmbH	Metronidazole	17290503	1
Caesar&Lorenz/AHD	Metronidazole	17290506	1
Caesar&Lorenz	Metronidazole	20004568003	2
Caesar&Lorenz	Metronidazole	21002293002	3
Caesar&Lorenz	Metronidazole	21002293003	1
Caesar&Loretz GmbH/Anzag	Metronidazole	12339511	1
Caesar&Loretz GmbH/S...	Metronidazole	15253003	1
Caesar&Loretz GmbH	Metronidazole	19000516019	1
Caesar&Loretz GmbH	Metronidazole	19010210	1
Caesar&Loretz GmbH	Metronidazole	21002293009	1
Caesar&loretz,Phoenix	Metronidazole	12110410	1
Cealo/ Gehe	Metronidazole	19010213	1
Cealo/Gehe	Metronidazole	17290506	1
cealo/Gehe	Metronidazole	20004568003	1
Cealo/Phoenix	Metronidazole	21002293011	1
Cealo/Sanacorp	Metronidazole	13095003	1
Cealo/Sanacorp	Metronidazole	1900051610	1
Cealo	Metronidazole	16089219	1
Cealo	Metronidazole	19000516001	1
Cealo	Metronidazole	20004568015	1
celo / Gehe	Metronidazole	123456	1
celo	Metronidazole	20004568003	3
Corden Pharma / Gehe	Metronidazole	17290504	1
Corden Pharma Bergam...	Metronidazole	C3356	1
Corden Pharma Bergamo S.p	Metronidazole	1807039-02	2
Corden Pharma Bergam...	Metronidazole	19010214	1
Corden Pharma Bergam...	Metronidazole	F180012	1
Corden Pharma	Metronidazole	1212001-02	2
Corden/ Gehe	Metronidazole	2207001-01	1
Corden/Noweda	Metronidazole	19010210	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Corden/Noweda	Metronidazole	F180029	1
Delta	Metronidazole	17058001	1
Delta	Metronidazole	17290503	2
E Plus	Metronidazole	1707008-01	1
Ebert & Jacobi	Metronidazole	1609028-01	2
Ebert	Metronidazole	1412016-02	1
Ebert-Jacobi	Metronidazole	16089224	1
Eu Rho	Metronidazole	2007002-02	1
EuRho / Noweda	Metronidazole	1807039-03	3
EuRho/AHD	Metronidazole	1906012-01	1
EuRho/Jenne	Metronidazole	1802007-02	1
EuRho/Noweda	Metronidazole	180601M1706022-01	1
EuRho/Noweda	Metronidazole	2007002-01	1
EuRho/Phoenix	Metronidazole	2007002-02	1
EuRho/Phönix	Metronidazole	1307002-01	1
EuRho	Metronidazole	110903002	1
EuRho	Metronidazole	1109030-02	1
EuRho	Metronidazole	1212001-02	1
EuRho	Metronidazole	1307042-02	1
Eurho	Metronidazole	1406010-01	1
EuRho	Metronidazole	1406010-01	1
EuRho	Metronidazole	1407003-01	1
EuRho	Metronidazole	1412016-01	1
eurho	Metronidazole	1612013-01	1
EuRho	Metronidazole	1612013-02	5
EuRho	Metronidazole	170103901	1
EuRho	Metronidazole	1701039-01	2
EuRho	Metronidazole	1706022-02	1
EuRho	Metronidazole	1707008-01	1
EuRho	Metronidazole	1802007-02	2
Eurho	Metronidazole	1807039-01	1
EuRho	Metronidazole	1807039-01	2
EuRho	Metronidazole	180703902	1
EuRho	Metronidazole	1807039-02	1
Eurho	Metronidazole	1908028-01	1
EuRho	Metronidazole	2005029-01	1
Eurimpharm	Metronidazole	140601001	1
EURO / Sanacorp	Metronidazole	160902801	1
Euro Gehe	Metronidazole	1707008-01	1
Euro OCT / Krieger	Metronidazole	1908028-02	1
Euro OTC	Metronidazole		4
Euro OTC	Metronidazole	10800401	1
Euro OTC	Metronidazole	1109016-01	1
Euro OTC	Metronidazole	1109030-01	5
Euro OTC	Metronidazole	110903002	1
Euro OTC	Metronidazole	1109030-02	1
Euro OTC	Metronidazole	1109030-03	2
Euro OTC	Metronidazole	1112028-01	4
Euro OTC	Metronidazole	1112028-02	7
Euro OTC	Metronidazole	121001-02	3
Euro OTC	Metronidazole	1212001-01	8
Euro OTC	Metronidazole	1212001-02	13
Euro OTC	Metronidazole	1212030-01	3
Euro OTC	Metronidazole	1212030-02	7
Euro OTC	Metronidazole	1220141155F	1
Euro OTC	Metronidazole	128061/72	1
Euro OTC	Metronidazole	13070002-02	1
Euro OTC	Metronidazole	1307002-01	11
Euro OTC	Metronidazole	1307002-02	1
Euro OTC	Metronidazole	130704201	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Metronidazole	1307042-01	9
Euro OTC	Metronidazole	1307042-02	7
Euro OTC	Metronidazole	1308704201	1
Euro OTC	Metronidazole	13214010	1
Euro OTC	Metronidazole	13B06-N03	1
Euro OTC	Metronidazole	140601001	2
Euro OTC	Metronidazole	1406010-01	21
Euro OTC	Metronidazole	1407003	1
Euro OTC	Metronidazole	140700301	1
Euro OTC	Metronidazole	1407003-01	7
Euro OTC	Metronidazole	140700302	2
Euro OTC	Metronidazole	1407003-02	10
Euro OTC	Metronidazole	1412016	1
Euro OTC	Metronidazole	1412016-01	15
Euro OTC	Metronidazole	1412016-02	26
Euro OTC	Metronidazole	14120601	1
Euro OTC	Metronidazole	1418E-01870	1
Euro OTC	Metronidazole	1503004-01	1
Euro OTC	Metronidazole	150502401	4
Euro OTC	Metronidazole	1505024-01	14
Euro OTC	Metronidazole	150502402	1
Euro OTC	Metronidazole	1505024-02	7
Euro OTC	Metronidazole	1505024-03	3
Euro OTC	Metronidazole	150800	1
Euro OTC	Metronidazole	1508004	1
Euro OTC	Metronidazole	150800401	1
Euro OTC	Metronidazole	1508004-01	27
Euro OTC	Metronidazole	1508004-02	13
Euro OTC	Metronidazole	150804-01	1
Euro OTC	Metronidazole	15a20-b07-303294	1
Euro OTC	Metronidazole	15A20-B07-308525	2
Euro OTC	Metronidazole	1606028	1
Euro OTC	Metronidazole	16089222	1
Euro OTC	Metronidazole	16089224	1
Euro OTC	Metronidazole	1609023-01	1
Euro OTC	Metronidazole	1609028	3
Euro OTC	Metronidazole	1609028-01	31
Euro OTC	Metronidazole	1609028-02	13
Euro OTC	Metronidazole	161201301	1
Euro OTC	Metronidazole	1612013-01	28
Euro OTC	Metronidazole	1612013-02	3
Euro OTC	Metronidazole	169028-01	1
Euro OTC	Metronidazole	1701039	2
Euro OTC	Metronidazole	170103901	1
Euro OTC	Metronidazole	1701039-01	57
Euro OTC	Metronidazole	170139-01	2
Euro OTC	Metronidazole	1703028-01	1
Euro OTC	Metronidazole	17058005	1
Euro OTC	Metronidazole	1706022_01	1
Euro OTC	Metronidazole	170602201	1
Euro OTC	Metronidazole	1706022-01	16
Euro OTC	Metronidazole	1706022-02	3
Euro OTC	Metronidazole	1707008-002	1
Euro OTC	Metronidazole	170700801	3
Euro OTC	Metronidazole	1707008-01	57
Euro OTC	Metronidazole	170700802	1
Euro OTC	Metronidazole	1707008-02	10
Euro OTC	Metronidazole	1707039-01	1
Euro OTC	Metronidazole	1707088-01	2
Euro OTC	Metronidazole	17290513	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Metronidazole	176022-01	1
Euro OTC	Metronidazole	180200701	1
Euro OTC	Metronidazole	1802007-01	14
Euro OTC	Metronidazole	1802007-02	4
Euro OTC	Metronidazole	1807030-01	1
Euro OTC	Metronidazole	1807031-01	1
Euro OTC	Metronidazole	1807039	2
Euro OTC	Metronidazole	1807039/01	1
Euro OTC	Metronidazole	1807039-01	40
Euro OTC	Metronidazole	180703902	1
Euro OTC	Metronidazole	1807039-02	33
Euro OTC	Metronidazole	1807039-03	20
Euro OTC	Metronidazole	19010210	1
Euro OTC	Metronidazole	190104201	3
Euro OTC	Metronidazole	1901042-01	14
Euro OTC	Metronidazole	190104202	1
Euro OTC	Metronidazole	1901042-02	11
Euro OTC	Metronidazole	190601201	1
Euro OTC	Metronidazole	1906012-01	29
Euro OTC	Metronidazole	1906012-02	23
Euro OTC	Metronidazole	1908028	3
Euro OTC	Metronidazole	190802801	1
Euro OTC	Metronidazole	1908028-01	10
Euro OTC	Metronidazole	190802802	1
Euro OTC	Metronidazole	1908028-02	16
Euro OTC	Metronidazole	1908028-1	1
Euro OTC	Metronidazole	20004568015	1
Euro OTC	Metronidazole	2005029-01	19
Euro OTC	Metronidazole	200502902	1
Euro OTC	Metronidazole	2005029-02	4
Euro OTC	Metronidazole	20070002-02	1
Euro OTC	Metronidazole	200700201	3
Euro OTC	Metronidazole	2007002-01	52
Euro OTC	Metronidazole	2007002-02	24
Euro OTC	Metronidazole	20111025	1
Euro OTC	Metronidazole	2103002-01	11
Euro OTC	Metronidazole	2103002-02	1
Euro OTC	Metronidazole	2103002-03	5
Euro OTC	Metronidazole	2206031-01	3
Euro OTC	Metronidazole	2207001_01	1
Euro OTC	Metronidazole	2207001-01	4
Euro OTC	Metronidazole	2308003-01	1
Euro OTC	Metronidazole	300915ME	1
Euro OTC	Metronidazole	4516E-01870	1
Euro OTC	Metronidazole	700837	1
Euro OTC	Metronidazole	C04-160812	1
Euro OTC	Metronidazole	C04-171127	1
Euro OTC	Metronidazole	F120017	1
Euro OTC	Metronidazole	F160028	1
Euro OTC	Metronidazole	F1800012	1
Euro OTC	Metronidazole	F190012	1
Euro OTC	Metronidazole	F200019	1
Euro/ Sanacorp	Metronidazole	150800402	1
Euro/Anzag	Metronidazole	1807039-02	1
Euro/Noweda	Metronidazole	1609028-01	1
Euro/Sanacorp	Metronidazole	1609028	1
EuroPharma	Metronidazole	141201601	1
EurRho/Noweda	Metronidazole	1908028-02	1
Fagro/Sanacorp	Metronidazole	18B28-B50	1
Fagro	Metronidazole	14C14-B01-295548	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Metronidazole		5
Fagron	Metronidazole	10F23-N05	1
Fagron	Metronidazole	112356	1
Fagron	Metronidazole	11C21-N01	1
Fagron	Metronidazole	11F15-N07	1
Fagron	Metronidazole	11J07-N07	1
Fagron	Metronidazole	1220141155F	2
Fagron	Metronidazole	12A20-B07-303298	1
Fagron	Metronidazole	12a2o-n18	1
Fagron	Metronidazole	12D30-N02	1
Fagron	Metronidazole	12d30-n03	1
Fagron	Metronidazole	12D30-N03	4
Fagron	Metronidazole	12f15-n04	1
Fagron	Metronidazole	12F15-N04	7
Fagron	Metronidazole	12G04-N15	15
Fagron	Metronidazole	12L17_N16	1
Fagron	Metronidazole	12l17-n11	1
Fagron	Metronidazole	12l17-N11	1
Fagron	Metronidazole	12L17N11	1
Fagron	Metronidazole	12L17-N11	15
Fagron	Metronidazole	12L17-N16	6
Fagron	Metronidazole	12L-N11	1
Fagron	Metronidazole	13/10-No3	1
Fagron	Metronidazole	13/21-N07	1
Fagron	Metronidazole	13/21-N7	2
Fagron	Metronidazole	13095002	1
Fagron	Metronidazole	13B06N03	1
Fagron	Metronidazole	13B06-N03	10
Fagron	Metronidazole	13D08N22	1
Fagron	Metronidazole	13D08-N22	6
Fagron	Metronidazole	13D10-N02	4
Fagron	Metronidazole	13I10-N03	3
Fagron	Metronidazole	13j21-n07	2
Fagron	Metronidazole	13j21-N07	1
Fagron	Metronidazole	13J21N07	2
Fagron	Metronidazole	13J21-N07	35
Fagron	Metronidazole	140700301	1
Fagron	Metronidazole	1412016-01	1
Fagron	Metronidazole	1414-B02-291237	1
Fagron	Metronidazole	141C14-B02-296437	1
Fagron	Metronidazole	14B27-B31-291234	1
Fagron	Metronidazole	14B27-B31-291235	1
Fagron	Metronidazole	14C12-B02-300182	1
Fagron	Metronidazole	14C14-802-291237	1
Fagron	Metronidazole	14C14-B01	1
Fagron	Metronidazole	14c14-B01-295545	1
Fagron	Metronidazole	14C14-B01-295548	1
Fagron	Metronidazole	14C14-B01-306363	5
Fagron	Metronidazole	14C14-B01-309058	2
Fagron	Metronidazole	14C14B02	3
Fagron	Metronidazole	14C14-B02	4
Fagron	Metronidazole	14C14-B02_291238	1
Fagron	Metronidazole	14C14-B02-2911239	1
Fagron	Metronidazole	14C14-B02-291237	9
Fagron	Metronidazole	14C14-B02-291238	2
Fagron	Metronidazole	14c14-b02-291239	1
Fagron	Metronidazole	14C14-B02-291239	7
Fagron	Metronidazole	14C14-B02-291241	1
Fagron	Metronidazole	14c14-b02-291275	1
Fagron	Metronidazole	14C14-B02-291275	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Metronidazole	14c14b02291276	1
Fagron	Metronidazole	14c14-b02-291276	2
Fagron	Metronidazole	14C14B02-291276	2
Fagron	Metronidazole	14C14-B02-291276	3
Fagron	Metronidazole	14C14-B02-295603	1
Fagron	Metronidazole	14C14-B02-296437	10
Fagron	Metronidazole	14-C14-B02-296437	1
Fagron	Metronidazole	14C14-B02-300182	4
Fagron	Metronidazole	14C14-B291237	1
Fagron	Metronidazole	14C14-Bo2-291276	1
Fagron	Metronidazole	1508004-01	1
Fagron	Metronidazole	15253017	2
Fagron	Metronidazole	15A20/B07-303298	1
Fagron	Metronidazole	15A20-B07	1
Fagron	Metronidazole	15A20-B07-303293	9
Fagron	Metronidazole	15A20-B07-303294	3
Fagron	Metronidazole	15A20-B07-303294Mg	1
Fagron	Metronidazole	15A20-B07-303295	1
Fagron	Metronidazole	15a20b07303298	1
Fagron	Metronidazole	15A20-B07-303298	8
Fagron	Metronidazole	15a20-b07-308196	1
Fagron	Metronidazole	15A20-B07-308196	3
Fagron	Metronidazole	15A20-B07-308198	1
Fagron	Metronidazole	15A20B07308525	1
Fagron	Metronidazole	15A20-B07-308525	6
Fagron	Metronidazole	15a20-b07-308791	1
Fagron	Metronidazole	15A20-B07-308791	4
Fagron	Metronidazole	15A20-B07312057	1
Fagron	Metronidazole	15A20-B07-312057	4
Fagron	Metronidazole	15A20-B07-312225	3
Fagron	Metronidazole	15A20-B07-31225	1
Fagron	Metronidazole	15A20Bo7308196	1
Fagron	Metronidazole	16/16-B04-326151	1
Fagron	Metronidazole	16/19-B04	3
Fagron	Metronidazole	16/19-B04-326150	6
Fagron	Metronidazole	16/19-B04-326151	3
Fagron	Metronidazole	16/19-B04-326152	1
Fagron	Metronidazole	16/19-B04-326154	1
Fagron	Metronidazole	16/19-B04-326155	2
Fagron	Metronidazole	16/19-B04-329160	1
Fagron	Metronidazole	16/19-B04-329162	1
Fagron	Metronidazole	16/19-B04-329163	1
Fagron	Metronidazole	16/19-B04-329167	2
Fagron	Metronidazole	16/19-b04-329168	1
Fagron	Metronidazole	16/19-B04-329168	3
Fagron	Metronidazole	16/19bo4326155	1
Fagron	Metronidazole	160902	1
Fagron	Metronidazole	1609028-01	2
Fagron	Metronidazole	1612013-01	3
Fagron	Metronidazole	1619-B04-326150	1
Fagron	Metronidazole	1619b04326155	1
Fagron	Metronidazole	1619-B04-326155	1
Fagron	Metronidazole	1619B04329161	1
Fagron	Metronidazole	16D15-B50-324137	2
Fagron	Metronidazole	16H15-B50-326734	1
Fagron	Metronidazole	16I19-B04	5
Fagron	Metronidazole	16I19-B04-326150	3
Fagron	Metronidazole	16I19-B04-326151	7
Fagron	Metronidazole	16I19-B04-326152	4
Fagron	Metronidazole	16I19-B04-326155	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Metronidazole	16I19-B04-329159	1
Fagron	Metronidazole	16I19-B04-329160	3
Fagron	Metronidazole	16I19-B04-329161	1
Fagron	Metronidazole	16I19-B04-329162	1
Fagron	Metronidazole	16I19-B04-329163	1
Fagron	Metronidazole	16I19-B04-329165	1
Fagron	Metronidazole	16I19-B04-329166	1
Fagron	Metronidazole	16I19-B04-329167	2
Fagron	Metronidazole	16I19-B04-329168	1
Fagron	Metronidazole	16J19B04	1
Fagron	Metronidazole	16J19-B04-326151	1
Fagron	Metronidazole	16J28-B50-329880	1
Fagron	Metronidazole	16L19_B04_326152	1
Fagron	Metronidazole	16l19-B04-326150	1
Fagron	Metronidazole	16l19-B04-329160	1
Fagron	Metronidazole	16l19-B04-329166	1
Fagron	Metronidazole	17/19-304-329168	1
Fagron	Metronidazole	17058003	1
Fagron	Metronidazole	17058013	1
Fagron	Metronidazole	172939-B01-295547	1
Fagron	Metronidazole	17A30-B01-335193	2
Fagron	Metronidazole	17A30-B0-335193	1
Fagron	Metronidazole	17C10	2
Fagron	Metronidazole	17C10-B04	6
Fagron	Metronidazole	17C-10-B04-338699	1
Fagron	Metronidazole	17C10-B04-338700	2
Fagron	Metronidazole	17C10-B04-338707	4
Fagron	Metronidazole	17C10-B04-346275	7
Fagron	Metronidazole	17c10-b04-346276	2
Fagron	Metronidazole	17C10-B04-346276	11
Fagron	Metronidazole	17C10-B04-346277	5
Fagron	Metronidazole	17C10-B04-346278	1
Fagron	Metronidazole	17C10-B04-346279	2
Fagron	Metronidazole	17C10-B04-346280	1
Fagron	Metronidazole	17C10-B04-355863	2
Fagron	Metronidazole	17C10-B04-355864	1
Fagron	Metronidazole	17C10-B04-355865	3
Fagron	Metronidazole	17C10-B04-355867	1
Fagron	Metronidazole	17C10-Bo4-346276	1
Fagron	Metronidazole	17C20-B04-355868	1
Fagron	Metronidazole	1802007-01	1
Fagron	Metronidazole	1802007-02	1
Fagron	Metronidazole	18026401	1
Fagron	Metronidazole	1807039-01	3
Fagron	Metronidazole	18B28-B50-354847	1
Fagron	Metronidazole	18B28B50354848	1
Fagron	Metronidazole	18B28-B50-354848	1
Fagron	Metronidazole	18B28-B50-354849	2
Fagron	Metronidazole	18B28-B50-354851	1
Fagron	Metronidazole	18B28-B50-354852	4
Fagron	Metronidazole	18B28-B50-3554852	1
Fagron	Metronidazole	1901042-01	1
Fagron	Metronidazole	19G002-B04-362813	1
Fagron	Metronidazole	19G02	1
Fagron	Metronidazole	19G02-B02-362815	1
Fagron	Metronidazole	19G02-B04	9
Fagron	Metronidazole	19G02-B04_362823	1
Fagron	Metronidazole	19G02-B04-362812	1
Fagron	Metronidazole	19G02B04362813	1
Fagron	Metronidazole	19G02-B04-362813	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Metronidazole	19G02B04362814	1
Fagron	Metronidazole	19G02-B04-362814	6
Fagron	Metronidazole	19G02-B04-362815	8
Fagron	Metronidazole	19G02-B04-362816	11
Fagron	Metronidazole	19G02-B04-362817	1
Fagron	Metronidazole	19G02-B04-362818	2
Fagron	Metronidazole	19G02-B04-362823	5
Fagron	Metronidazole	19G02-B04-367358	1
Fagron	Metronidazole	19G02-B04-367359	2
Fagron	Metronidazole	19G02-B04-367360	1
Fagron	Metronidazole	19G02-B04-367363	2
Fagron	Metronidazole	19G02-B04-36763	1
Fagron	Metronidazole	19GO2-BO4-362814	1
Fagron	Metronidazole	19119-B04-326154	1
Fagron	Metronidazole	20007-F03-0003	1
Fagron	Metronidazole	20121121	3
Fagron	Metronidazole	20130906F	4
Fagron	Metronidazole	20140131f	1
Fagron	Metronidazole	20140131F	3
Fagron	Metronidazole	20G07_F03-372291	1
Fagron	Metronidazole	20g07-f03	1
Fagron	Metronidazole	20G07-F03	8
Fagron	Metronidazole	20G07-F03_372291	1
Fagron	Metronidazole	20G07F03372286	1
Fagron	Metronidazole	20G07-F03-372286	7
Fagron	Metronidazole	20g07-f03-372287	2
Fagron	Metronidazole	20G07-F03-372287	3
Fagron	Metronidazole	20G07-F03-372288	1
Fagron	Metronidazole	20G07-F03-372290	1
Fagron	Metronidazole	20G07-F03-372291	17
Fagron	Metronidazole	20G07-F3-372288	1
Fagron	Metronidazole	21G29-B02	1
Fagron	Metronidazole	21G29-B02-213325	12
Fagron	Metronidazole	21G29-B02-213328	1
Fagron	Metronidazole	21G29-B02-221569	1
Fagron	Metronidazole	21G29-B02-221570	1
Fagron	Metronidazole	220401M	1
Fagron	Metronidazole	2OG07-FO3-372291	1
Fagron	Metronidazole	3212E01870	1
Fagron	Metronidazole	443-48-1	1
Fagron	Metronidazole	48(17C10-B04-346277	1
Fagron	Metronidazole	601021826	2
Fagron	Metronidazole	601062027	4
Fagron	Metronidazole	601072127	1
Fagron	Metronidazole	603041926	4
Fagron	Metronidazole	604081626	6
Fagron	Metronidazole	605021726	4
Fagron	Metronidazole	606/10072017	1
Fagron	Metronidazole	61021826	1
Fagron	Metronidazole	700837-0008	1
Fagron	Metronidazole	700837-B04-367361	1
Fagron	Metronidazole	9041303	1
Fagron	Metronidazole	B04-3628104	1
Fagron	Metronidazole	B04-3628106	2
Fagron	Metronidazole	B04-3673509	1
Fagron	Metronidazole	F03-3722806	2
Fagron	Metronidazole	F03-3722807	1
Fagron	Metronidazole	F03-3722808	1
Fagron	Metronidazole	Metr23012023	1
Fagron	Metronidazole	PM41	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Farchemia / Gehe	Metronidazole	15253017	1
Farchemia S. r. l.	Metronidazole	1609028-01	1
Farchemia S.R.L./ Ca...	Metronidazole	15253032	1
Farchemia/Phönix	Metronidazole	1609028-02	1
Fargon	Metronidazole	13D08-N22	1
Fargon	Metronidazole	14c14-b02-291238	1
Fargon	Metronidazole	19G02-B04-367360	1
Fargon	Metronidazole	21G29-B02-213325	1
Fiebig	Metronidazole	16089235	1
Fiebig	Metronidazole	17058005	1
Fiebig	Metronidazole	17058027	1
Fiebig	Metronidazole	17290504	2
Fiebig	Metronidazole	17290506	1
Fiebig	Metronidazole	17290507	1
Fiebig	Metronidazole	17290517	2
Fiebig	Metronidazole	17290527	1
Fiebig	Metronidazole	17290532	1
Fiebig	Metronidazole	b04-3673509	1
Fiebig	Metronidazole	B04-3673509	1
Fischer/Gehe	Metronidazole	15A20-B07-308525	1
Frago/Noweda	Metronidazole	16I19-B04-329163	1
Fragon/Jenne	Metronidazole	19Go2-B04-367359	1
Gatt-Koller	Metronidazole	3728/11162017	1
Gatt-Koller	Metronidazole	497/03151015	1
Gatt-Koller	Metronidazole	497/03151515	1
Gatt-Koller	Metronidazole	497/03154015	1
Gatt-Koller	Metronidazole	606293914	1
GEHE 11.06.2014	Metronidazole	1307002-01	1
Gehe 23.11.18	Metronidazole	1706022-02	1
Gehe am 04.02.14	Metronidazole	1212030-01	2
Gehe amax	Metronidazole	17058012	1
Gehe amax	Metronidazole	17290506	1
Gehe amax	Metronidazole	17290507	2
Gehe amax	Metronidazole	17290533	1
Gehe amax	Metronidazole	1807039-03	1
Gehe amax	Metronidazole	19000516002	1
Gehe amax	Metronidazole	1908028-02	1
Gehe Rostock	Metronidazole	1906012-01	1
Gehe	Metronidazole	10368318	1
Gehe	Metronidazole	1112028-02	1
Gehe	Metronidazole	12110415	1
Gehe	Metronidazole	12110422	1
Gehe	Metronidazole	1307002-01	1
Gehe	Metronidazole	1307002-02	1
Gehe	Metronidazole	140700301	1
Gehe	Metronidazole	1407003-01	2
Gehe	Metronidazole	1505024-01	1
Gehe	Metronidazole	15215108	1
Gehe	Metronidazole	15253017	1
Gehe	Metronidazole	15253026	1
Gehe	Metronidazole	15253032	1
GEHE	Metronidazole	15253032	1
GEHE	Metronidazole	16089216	1
GEHE	Metronidazole	16089229	1
Gehe	Metronidazole	16H15-B50-326734	1
GEHE	Metronidazole	17058013	1
GEHE	Metronidazole	17058015	1
Gehe	Metronidazole	17058016	2
Gehe	Metronidazole	17058019	1
Gehe	Metronidazole	1707008	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Metronidazole	17290506	1
Gehe	Metronidazole	17290518	1
Gehe	Metronidazole	1802007-01	1
Gehe	Metronidazole	19000516006	1
Gehe	Metronidazole	19000516008	1
Gehe	Metronidazole	190102003	1
Gehe	Metronidazole	19G02-B04-362813	2
Gehe	Metronidazole	20004568009	1
Gehe	Metronidazole	2005029-02	1
Gehe	Metronidazole	2007002-01	1
Gehe	Metronidazole	2007002-02	1
Gehe	Metronidazole	20140131F	1
Gehe	Metronidazole	21002293020	1
GEHE	Metronidazole	22002266007	1
Gehe	Metronidazole	22002266008	1
Gehe	Metronidazole	220631-01	1
Gehe	Metronidazole	60106207	1
Gehe	Metronidazole	F03-3722806	2
Gehe01/2018	Metronidazole	14C14-B02-291237	1
Geilenkirchen	Metronidazole	13214018	1
Geilenkirchen	Metronidazole	16089222	1
Geilenkirchen	Metronidazole	1807039-03	1
GH: ...	Metronidazole	17290503	1
GUMO	Metronidazole	2007002-01	1
GUMO	Metronidazole	2007002-02	3
Hedinger/Noweda	Metronidazole	166089220	1
Henry Lamotte	Metronidazole	1212001-02	1
Herberata Arzneimittel	Metronidazole	15253024I-02082016	1
Hubei Hongyuan	Metronidazole	140700301	1
Ichthyol Gesellschaft	Metronidazole	13095005	1
Ichthyol/ALH	Metronidazole	1609028-02	1
Infectopharm / Alliance	Metronidazole	18B28-B50-354849	1
Jenne	Metronidazole	21002293006	1
Jenne	Metronidazole	22002266002	1
Jenne	Metronidazole	22002266008	1
Jenne	Metronidazole	24000389003	1
Kehr	Metronidazole	17058003	1
Kehr	Metronidazole	17290512	1
Kehr	Metronidazole	2007002-02	1
Kehr	Metronidazole	21002293020	1
Kehr	Metronidazole	2207001-01	1
Klosterring	Metronidazole	16089235	1
krieger	Metronidazole	19010203	1
Kuerzel	Metronidazole	1307002-02	1
L10	Metronidazole	1807039-01	4
L12	Metronidazole	1609028-01	1
L12	Metronidazole	1609028-02	1
L30	Metronidazole	16089224	2
Laborch.Apolda/Gehe	Metronidazole	17C10_B04_346278	1
Noweda /Cealo	Metronidazole	19000516016	1
Noweda 19.12.22 EK 6,37	Metronidazole	21002293014	2
Noweda 27.11.2019	Metronidazole	19010211	1
Noweda/Wepa	Metronidazole	13214017	1
Noweda	Metronidazole	11319818	1
Noweda	Metronidazole	12110404	1
Noweda	Metronidazole	12339501	1
Noweda	Metronidazole	12G04-N15	1
Noweda	Metronidazole	13095012	1
Noweda	Metronidazole	13214025	1
Noweda	Metronidazole	1407003-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Metronidazole	1505024-03	1
Noweda	Metronidazole	160902802	1
Noweda	Metronidazole	1619-B04-329166	1
Noweda	Metronidazole	1701039-01	1
Noweda	Metronidazole	17058004	2
Noweda	Metronidazole	17058005	2
Noweda	Metronidazole	17058013	1
Noweda	Metronidazole	17058014	2
Noweda	Metronidazole	1706022-01	1
Noweda	Metronidazole	1707008-01	2
Noweda	Metronidazole	17290518	1
Noweda	Metronidazole	17290519	1
Noweda	Metronidazole	17290526	1
Noweda	Metronidazole	17290532	1
Noweda	Metronidazole	1807039-02	1
Noweda	Metronidazole	1807039-03	1
Noweda	Metronidazole	19000516019	1
Noweda	Metronidazole	19010212	1
Noweda	Metronidazole	19G02-B04-362814	1
Noweda	Metronidazole	20004568015	1
Noweda	Metronidazole	200700201	1
Noweda	Metronidazole	2007002-01	3
Noweda	Metronidazole	2007002-02	2
noweda	Metronidazole	2100223016	1
Noweda	Metronidazole	21002293016	1
Noweda	Metronidazole	21002293017	1
Noweda	Metronidazole	21002293019	1
Noweda	Metronidazole	21002293020	1
Noweda	Metronidazole	22002266004	2
Noweda	Metronidazole	22002266006	1
Noweda	Metronidazole	2206031-01	2
Noweda	Metronidazole	2207001-01	1
Noweda	Metronidazole	2308004-01	1
Otto Fischar GmbH&Co KG	Metronidazole	17058017	1
Phoenix 11.09.13	Metronidazole	12L17-N11	1
Phoenix 11.05.2017 6,59EUR	Metronidazole	16089220	1
Phoenix 12.10.2016 6,63EUR	Metronidazole	15253027	1
Phoenix 15.05.18 6,52EUR	Metronidazole	17058017	1
Phoenix 4.3.2019	Metronidazole	17290526	1
Phoenix/Cealo	Metronidazole	17058016/0818E-0187	1
Phoenix	Metronidazole		1
Phoenix	Metronidazole	121203002	1
Phoenix	Metronidazole	15253032	1
Phoenix	Metronidazole	16089201	1
Phoenix	Metronidazole	16089224	1
Phoenix	Metronidazole	17058002	1
Phoenix	Metronidazole	17058013	1
Phoenix	Metronidazole	17058026	1
Phoenix	Metronidazole	17058027	1
Phoenix	Metronidazole	17290517	1
Phoenix	Metronidazole	17290527	2
Phoenix	Metronidazole	19010202	2
Phoenix	Metronidazole	19010216	1
phoenix	Metronidazole	1908028-02	2
Phoenix	Metronidazole	20004568009	1
Phoenix	Metronidazole	200490406	1
Phoenix	Metronidazole	21002293020	2
Phoenix	Metronidazole	22002266002	2
Phoenix	Metronidazole	3403	1
Phönix Gotha	Metronidazole	13214017	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix Gotha	Metronidazole	17058018	1
Phönix/ Corden Pharm…	Metronidazole	17290518	1
Phönix	Metronidazole	1109030-03	1
Phönix	Metronidazole	121203001	1
Phönix	Metronidazole	12L17-N11	1
Phönix	Metronidazole	13214017	2
Phönix	Metronidazole	13J21-N07	1
Phönix	Metronidazole	15253018	1
phönix	Metronidazole	15253026	1
Phönix	Metronidazole	16089212	1
Phönix	Metronidazole	16089223	1
Phonix	Metronidazole	1612013-01	1
Phönix	Metronidazole	1701039-01	1
Phönix	Metronidazole	17058003	1
Phönix	Metronidazole	17058005	1
PHÖNIX	Metronidazole	17058011	3
Phönix	Metronidazole	17058016	1
Phönix	Metronidazole	1707008-01	1
Phönix	Metronidazole	172905070	1
Phönix	Metronidazole	17290527	1
Phönix	Metronidazole	17290532	1
Phönix	Metronidazole	18026401	1
Phönix	Metronidazole	1807039-01	2
Phönix	Metronidazole	19000516010	2
Phönix	Metronidazole	19010210	1
Phönix	Metronidazole	19010214	1
Phönix	Metronidazole	200700201	1
Phönix	Metronidazole	2007002-01	1
Phönix	Metronidazole	20G07-F03-372286	1
Phönix	Metronidazole	21002293020	2
Phönix	Metronidazole	22002266008	1
Phönix	Metronidazole	2200226606	1
Phönix	Metronidazole	22602266006	1
Phönix	Metronidazole	3179	1
PHÖNIX	Metronidazole	601062027	1
Phönix	Metronidazole	Mez5	1
Phönix_13.12.2018	Metronidazole	17290518	1
Pohlpharma/Noweda	Metronidazole	601062027	3
Polpharma Pharmaceut…	Metronidazole	16I19-B04-326151	1
Polpharma/Noweda	Metronidazole	603041926	1
Reichelt	Metronidazole	17058013	1
Röntgen	Metronidazole	1906012-01	1
Röntgen	Metronidazole	F190012	1
Sana	Metronidazole	19010210	1
Sanacorp 27.10.15	Metronidazole	15A20-B07-303298	1
Sanacorp 02.03.15	Metronidazole	13214009	1
Sanacorp	Metronidazole		1
Sanacorp	Metronidazole	12110422	1
Sanacorp	Metronidazole	12339519	1
Sanacorp	Metronidazole	12G04-N15	1
Sanacorp	Metronidazole	13095002	1
Sanacorp	Metronidazole	16G02-B04-367358	1
Sanacorp	Metronidazole	16I19-B04-329159	1
Sanacorp	Metronidazole	16I19-B04-329160	1
Sanacorp	Metronidazole	1701039-01	1
Sanacorp	Metronidazole	17058002	1
Sanacorp	Metronidazole	17058014	1
Sanacorp	Metronidazole	17058018	1
Sanacorp	Metronidazole	1707008-01	2
Sanacorp	Metronidazole	17290512	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Metronidazole	17290518	1
Sanacorp	Metronidazole	17290525	1
Sanacorp	Metronidazole	17290526	1
Sanacorp	Metronidazole	17290533	2
Sanacorp	Metronidazole	17C10-B04-338707	1
Sanacorp	Metronidazole	17C10-B04-346280	2
Sanacorp	Metronidazole	19000516003	2
Sanacorp	Metronidazole	19010201	1
Sanacorp	Metronidazole	19010211	1
Sanacorp	Metronidazole	1906012-01	1
Sanacorp	Metronidazole	20004568003	2
Sanacorp	Metronidazole	20004568008	1
sanacorp	Metronidazole	200700201	1
Sanacorp	Metronidazole	20G07-F03	2
Sanacorp	Metronidazole	20G07-F03-372286	1
Sanacorp	Metronidazole	21002293020	1
Sanacorp	Metronidazole	21G29-B02-213325	1
Sanacorp	Metronidazole	22002266008	2
Sanacorp	Metronidazole	2206031-01	2
Sanacorp	Metronidazole	39/AKD18	1
Sanacorp	Metronidazole	39/AKD6	1
Sanacorp	Metronidazole	39AKD15	1
Sanacorp	Metronidazole	601021826	1
Sanacorp	Metronidazole	605021726	1
Sanacorp	Metronidazole	F200019	1
Spangro 28.05.2014	Metronidazole	13/10-N03	1
Spangropharm	Metronidazole	11319818	1
synthetisch	Metronidazole	2007002-02	1
test	Metronidazole		1
vdl	Metronidazole	12110421	1
WE Alliance Healthca...	Metronidazole	19010201	1
WEPA/Gehe	Metronidazole	20180515-04P	1

- 230 612 spectra from 1515 *Apo-Ident* customers from a total of 48 491 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Metronidazole* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Metronidazole* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	1130	0	200 954
Type C	0	5323	132	230 612

The substance/substance group *Metronidazole* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4690 %)
Type C	100.0000 % (> 99.9007 %)	97.5802 % (> 97.5252 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20857	21881	7.92	132.19
21212	22472	7.57	130.07
21213	22472	6.59	129.63
21356	21881	5.39	132.59
21360	22472	4.69	132.37
21881	21881	0.00	131.61
22472	22472	0.00	131.94
22835	22472	2.65	131.90
25330	25330	0.00	127.64
25565	25565	0.00	131.61

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Miconazole nitrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20210-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Miconazole nitrate; Miconazoli nitras

Special notes

When selecting the *Miconazole nitrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Miconazole nitrate	7	16	477

Second-stage model

For differentiation of the substance/substance group *Miconazole nitrate* the following second-stage model is used:

- Submodel 12

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Miconazole nitrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	148.51	–
⋮	⋮	⋮
Mesalazine	>50	65.94
Clioquinol	>50	118.15
Nicotinic acid	>50	160.79
Theophylline-ethylenediamine hydrate	>50	253.84

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Miconazole nitrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Miconazole nitrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Miconazole nitrate	13185601	20875	40	20130704
Caelo	Miconazole nitrate	13185601	20905	80	20130704
Caelo	Miconazole nitrate	13352802	21350	39	1412250
Caelo	Miconazole nitrate	13352802	21351	40	20131118
Caelo	Miconazole nitrate	161447	22630	40	20160617*
Euro OTC	Miconazole nitrate	1307025-02	21649	60	20130806
Euro OTC	Miconazole nitrate	1509014	21900	60	20150930*
Fagron	Miconazole nitrate	13D22-N14	20817	100	20130529
Fagron	Miconazole nitrate	18C23-B02-356141	24593	40	20180416

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 499 spectra of 9 reference samples from the substance/substance group *Miconazole nitrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 463 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 670 spectra of 18 reference samples from the substance/substance group *Miconazole nitrate*.

- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Miconazole nitrate	172175	23662	30
Caelo	Miconazole nitrate	182821	24388	40
Caelo	Miconazole nitrate	21000827011	26621	40
Euro OTC	Miconazole nitrate	1604004	22522	40
Euro OTC	Miconazole nitrate	1607004	22671	40
Euro OTC	Miconazole nitrate	1611024	22920	40
Euro OTC	Miconazole nitrate	1705039	23429	40
Euro OTC	Miconazole nitrate	1710020	23775	40
Euro OTC	Miconazole nitrate	1803028	24071	40
Euro OTC	Miconazole nitrate	1811015	24338	40
Euro OTC	Miconazole nitrate	1904032	24601	40
Euro OTC	Miconazole nitrate	1909029	24938	40
Euro OTC	Miconazole nitrate	2009034	25417	40
Euro OTC	Miconazole nitrate	2103012	25676	40
Euro OTC	Miconazole nitrate	2210002	26427	40
Fagron	Miconazole nitrate	22F08-B02-221067	26173	40
Caelo	Miconazole nitrate	21000827011	26621SI	20
Fagron	Miconazole nitrate	22F08-B02-221067	26173SI	20

- 201 414 spectra from a total of 4029 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3256 spectra from 843 *Apo-Ident* customers from 510 batches from the substance/substance group *Miconazole nitrate*.
- Among them are spectra of independent samples from 475 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Miconazole nitrate	2009034-02	1
	Miconazole nitrate	210008270022	1
	Miconazole nitrate	21000827013	1
	Miconazole nitrate	21000827016	4
	Miconazole nitrate	21000827017	2
	Miconazole nitrate	21000827018	2
	Miconazole nitrate	21000827019	1
	Miconazole nitrate	21000827021	1
	Miconazole nitrate	21000827022	3
	Miconazole nitrate	21000827023	7
	Miconazole nitrate	21000827024	4
	Miconazole nitrate	21000827025	9
	Miconazole nitrate	21000827026	10
	Miconazole nitrate	2100087024	1
	Miconazole nitrate	2103012-02	1
	Miconazole nitrate	2210002	1
	Miconazole nitrate	2210002-0	1
	Miconazole nitrate	2210002-01	10
	Miconazole nitrate	22832-87-7	1
	Miconazole nitrate	22F08-B02-213149	1
	Miconazole nitrate	22F08-B02-213580	1
	Miconazole nitrate	22F08-B02-221067	3
	Miconazole nitrate	23000589001	3
	Miconazole nitrate	23000589003	3
	Miconazole nitrate	23000589004	8
	Miconazole nitrate	23003273002	1
	Miconazole nitrate	23003273006	1
	Miconazole nitrate	2300589001	1
	Miconazole nitrate	2311020-01	2
	Miconazole nitrate	B02-221067	1
	Miconazole nitrate	B09-2402706	1
18282105	Miconazole nitrate	8704870	1
18282114	Miconazole nitrate	CAELO	1
20; 04.12.13	Miconazole nitrate	13185611	2
AEP	Miconazole nitrate	21000827019	1
AHC	Miconazole nitrate	23000589004	1
AHD	Miconazole nitrate	12374307	1
AHD	Miconazole nitrate	21000827018	1
AHD	Miconazole nitrate	23003273004	2
Alliance H.	Miconazole nitrate	5137910	1
Alliance Health 05.0...	Miconazole nitrate	13352801	2
Alliance Healthcare	Miconazole nitrate	12374307	1
Alliance Healthcare	Miconazole nitrate	1811015-01	2
Alliance Healthcare	Miconazole nitrate	18C23-B02-353243	1
Alliance Healthcare	Miconazole nitrate	18C23-B02-355295	1
Alliance	Miconazole nitrate	22F08-B02-213149	1
Anzag	Miconazole nitrate	12243802	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Anzag	Miconazole nitrate	12374301	3
Anzag	Miconazole nitrate	15137902	1
Anzag	Miconazole nitrate	15A13-B07-308432	1
Anzag	Miconazole nitrate	16144716	1
Anzag	Miconazole nitrate	18C23-B02-353243	1
Bionorica /Phönix	Miconazole nitrate	12C13B03-279593	1
Bomastus / Alliance ...	Miconazole nitrate	16E04-B03-327367	1
Bombastus	Miconazole nitrate	13352806	1
Bombastus	Miconazole nitrate	15I08-B07-318686	1
Bombastus	Miconazole nitrate	15I08-B07-318687	1
Bombastus	Miconazole nitrate	16144725	1
Caelo	Miconazole nitrate		3
Caelo	Miconazole nitrate	1/AD1	1
Caelo	Miconazole nitrate	11104103	2
Caelo	Miconazole nitrate	11104108	1
Caelo	Miconazole nitrate	11104109	2
Caelo	Miconazole nitrate	11104113	1
Caelo	Miconazole nitrate	11104114	1
Caelo	Miconazole nitrate	1122014A	1
Caelo	Miconazole nitrate	11243803	1
Caelo	Miconazole nitrate	11324901	1
Caelo	Miconazole nitrate	11324902	1
Caelo	Miconazole nitrate	11324905	4
Caelo	Miconazole nitrate	11324909	1
Caelo	Miconazole nitrate	11324912	2
Caelo	Miconazole nitrate	11324913	1
Caelo	Miconazole nitrate	122438	1
Caelo	Miconazole nitrate	12243801	3
Caelo	Miconazole nitrate	12243802	4
Caelo	Miconazole nitrate	12243803	9
Caelo	Miconazole nitrate	12243805	6
Caelo	Miconazole nitrate	12243806	1
Caelo	Miconazole nitrate	12243808	9
Caelo	Miconazole nitrate	12374301	4
Caelo	Miconazole nitrate	12374307	15
Caelo	Miconazole nitrate	12374308	6
Caelo	Miconazole nitrate	12k02n06	1
Caelo	Miconazole nitrate	1307025-02	1
Caelo	Miconazole nitrate	13185601	4
Caelo	Miconazole nitrate	13185602	7
Caelo	Miconazole nitrate	13185603	10
Caelo	Miconazole nitrate	13185609	9
Caelo	Miconazole nitrate	13185610	6
Caelo	Miconazole nitrate	13185611	16
Caelo	Miconazole nitrate	13185612	6
Caelo	Miconazole nitrate	13282901	1
Caelo	Miconazole nitrate	13342801	1
Caelo	Miconazole nitrate	13352801	17
Caelo	Miconazole nitrate	13352802	17
Caelo	Miconazole nitrate	13352805	1
Caelo	Miconazole nitrate	13352806	14
Caelo	Miconazole nitrate	13352811	6
Caelo	Miconazole nitrate	13D22-N14	1
Caelo	Miconazole nitrate	13H28-N06	1
Caelo	Miconazole nitrate	14149301	14
Caelo	Miconazole nitrate	14149302	16
Caelo	Miconazole nitrate	14149303	5
Caelo	Miconazole nitrate	14149305	1
Caelo	Miconazole nitrate	14149308	11
Caelo	Miconazole nitrate	14149309	9

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Miconazole nitrate	14149310	9
Caelo	Miconazole nitrate	14149311	14
Caelo	Miconazole nitrate	14149317	10
Caelo	Miconazole nitrate	14149318	22
Caelo	Miconazole nitrate	1419301	1
Caelo	Miconazole nitrate	1419310	1
Caelo	Miconazole nitrate	14B18-B02-291233	1
Caelo	Miconazole nitrate	14D25-B06-294959	1
Caelo	Miconazole nitrate	14D25-B06-294960	3
Caelo	Miconazole nitrate	14H06-B01-299799	1
Caelo	Miconazole nitrate	15/05-B07-312317	1
Caelo	Miconazole nitrate	15/08-B07-315481	1
Caelo	Miconazole nitrate	151379	1
Caelo	Miconazole nitrate	15137902	24
Caelo	Miconazole nitrate	15137903	19
Caelo	Miconazole nitrate	15137905	11
Caelo	Miconazole nitrate	15137906	1
Caelo	Miconazole nitrate	15137907	13
Caelo	Miconazole nitrate	15137908	10
Caelo	Miconazole nitrate	15137909	13
Caelo	Miconazole nitrate	15137910	7
Caelo	Miconazole nitrate	15137911	1
Caelo	Miconazole nitrate	15137913	5
Caelo	Miconazole nitrate	15137914	6
Caelo	Miconazole nitrate	15137915	3
Caelo	Miconazole nitrate	15A13-B07	1
Caelo	Miconazole nitrate	15A13-B07-307140	1
Caelo	Miconazole nitrate	15I08-B07-312317	3
Caelo	Miconazole nitrate	15I08-B07-315481	1
Caelo	Miconazole nitrate	15I08-B07-315492	1
Caelo	Miconazole nitrate	15I08-B07-318687	2
Caelo	Miconazole nitrate	15l08-B07-314838	1
Caelo	Miconazole nitrate	15l08-B07-315492	1
Caelo	Miconazole nitrate	15l08-B07-318686	1
Caelo	Miconazole nitrate	16144701	35
Caelo	Miconazole nitrate	16144702	27
Caelo	Miconazole nitrate	16144703	17
Caelo	Miconazole nitrate	16144704	14
Caelo	Miconazole nitrate	1614471	1
Caelo	Miconazole nitrate	16144710	17
Caelo	Miconazole nitrate	16144711	14
Caelo	Miconazole nitrate	16144716	30
Caelo	Miconazole nitrate	16144717	10
Caelo	Miconazole nitrate	16144720	10
Caelo	Miconazole nitrate	16144721	15
Caelo	Miconazole nitrate	16144725	38
Caelo	Miconazole nitrate	16144726	21
Caelo	Miconazole nitrate	16e04-b03-321367	1
Caelo	Miconazole nitrate	16E04-B03-321367	2
Caelo	Miconazole nitrate	16E04-B03-322124	1
Caelo	Miconazole nitrate	16E04-B03-325448	1
Caelo	Miconazole nitrate	16e04b03327367	1
Caelo	Miconazole nitrate	16E04-B03-332373	1
Caelo	Miconazole nitrate	1705039-01	2
Caelo	Miconazole nitrate	172117505	1
Caelo	Miconazole nitrate	1721505	1
Caelo	Miconazole nitrate	17217053	1
Caelo	Miconazole nitrate	17217502	52
Caelo	Miconazole nitrate	17217503	27
Caelo	Miconazole nitrate	17217505	32

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Miconazole nitrate	17217507	1
Caelo	Miconazole nitrate	1727503	1
Caelo	Miconazole nitrate	17C01B02340778	1
Caelo	Miconazole nitrate	180057913	1
Caelo	Miconazole nitrate	1803028-01	1
Caelo	Miconazole nitrate	18057901	1
Caelo	Miconazole nitrate	18057902	18
Caelo	Miconazole nitrate	18057903	29
Caelo	Miconazole nitrate	18057904	1
Caelo	Miconazole nitrate	18057906	38
Caelo	Miconazole nitrate	18057907	20
Ĉaelo	Miconazole nitrate	18057907	1
Caelo	Miconazole nitrate	18057909	1
Caelo	Miconazole nitrate	18057911	1
Caelo	Miconazole nitrate	18057912	29
Caelo	Miconazole nitrate	18057913	34
Caelo	Miconazole nitrate	18057914	16
Caelo	Miconazole nitrate	18057916	1
Caelo	Miconazole nitrate	18067907	1
Caelo	Miconazole nitrate	1807902	1
Caelo	Miconazole nitrate	18182111	1
Caelo	Miconazole nitrate	1828109	1
Caelo	Miconazole nitrate	1828113	3
Caelo	Miconazole nitrate	182821002	1
Caelo	Miconazole nitrate	18282101	2
Caelo	Miconazole nitrate	18282105	32
Caelo	Miconazole nitrate	18282106	15
Caelo	Miconazole nitrate	18282107	2
Caelo	Miconazole nitrate	18282108	2
Caelo	Miconazole nitrate	18282109	29
Caelo	Miconazole nitrate	18282110	27
Caelo	Miconazole nitrate	18282111	29
Caelo	Miconazole nitrate	18282113	62
Caelo	Miconazole nitrate	18282114	19
Caelo	Miconazole nitrate	1828213	1
Caelo	Miconazole nitrate	18282133	1
Caelo	Miconazole nitrate	1850000164	3
Caelo	Miconazole nitrate	1882105	1
Caelo	Miconazole nitrate	18B06_b03_34778	1
Caelo	Miconazole nitrate	18B06-B03-347788	1
Caelo	Miconazole nitrate	18C23-B02	2
Caelo	Miconazole nitrate	18C23-B02-348857	2
Caelo	Miconazole nitrate	18C23-B02-352488	1
Caelo	Miconazole nitrate	18C23-B02-353243	1
Caelo	Miconazole nitrate	18C23-B02-355707	1
Caelo	Miconazole nitrate	19A31-B01-359396	3
Caelo	Miconazole nitrate	19A31-B01-360614	2
Caelo	Miconazole nitrate	200000097003	2
Caelo	Miconazole nitrate	20000097001	1
Caelo	Miconazole nitrate	20000097003	30
Caelo	Miconazole nitrate	20000097004	19
Caelo	Miconazole nitrate	20000097005	7
Caelo	Miconazole nitrate	20000097006	13
Caelo	Miconazole nitrate	20000097007	30
Caelo	Miconazole nitrate	20000097009	1
Caelo	Miconazole nitrate	2000009705	1
Caelo	Miconazole nitrate	2000009707	1
Caelo	Miconazole nitrate	200004304002	1
Caelo	Miconazole nitrate	200004304003	1
Caelo	Miconazole nitrate	2000097003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Miconazole nitrate	2000097007	1
Caelo	Miconazole nitrate	20001304002	1
Caelo	Miconazole nitrate	20004304001	1
Caelo	Miconazole nitrate	20004304002	18
Caelo	Miconazole nitrate	20004304003	44
Caelo	Miconazole nitrate	20004304004	1
Caelo	Miconazole nitrate	20004304006	3
Caelo	Miconazole nitrate	2004304002	2
Caelo	Miconazole nitrate	2004304003	1
Caelo	Miconazole nitrate	2100027013	1
Caelo	Miconazole nitrate	21000827	1
Caelo	Miconazole nitrate	21000827001	2
Caelo	Miconazole nitrate	21000827002	14
Caelo	Miconazole nitrate	21000827003	49
Caelo	Miconazole nitrate	21000827006	12
Caelo	Miconazole nitrate	21000827007	3
Caelo	Miconazole nitrate	21000827008	24
Caelo	Miconazole nitrate	21000827010	5
Caelo	Miconazole nitrate	21000827011	7
Caelo	Miconazole nitrate	21000827012	5
Caelo	Miconazole nitrate	21000827013	15
Caelo	Miconazole nitrate	21000827014	19
Caelo	Miconazole nitrate	21000827015	9
Caelo	Miconazole nitrate	21000827016	7
Caelo	Miconazole nitrate	21000827017	6
Caelo	Miconazole nitrate	21000827019	4
Caelo	Miconazole nitrate	21000827021	3
Caelo	Miconazole nitrate	21000827022	5
Caelo	Miconazole nitrate	21000827023	1
Caelo	Miconazole nitrate	21000827024	5
Caelo	Miconazole nitrate	21000827025	1
Caelo	Miconazole nitrate	21000827026	3
Caelo	Miconazole nitrate	21000827103	1
Caelo	Miconazole nitrate	2100827002	1
Caelo	Miconazole nitrate	2100827003	1
Caelo	Miconazole nitrate	2100827008	2
Caelo	Miconazole nitrate	2100827014	1
Caelo	Miconazole nitrate	2100827019	1
Caelo	Miconazole nitrate	2103012-01	3
Caelo	Miconazole nitrate	211019(20004304002)	1
Caelo	Miconazole nitrate	211020(21000827002)	1
Caelo	Miconazole nitrate	21C09-F01-377510	1
Caelo	Miconazole nitrate	21C09-F01-3775100	2
Caelo	Miconazole nitrate	220004304003	1
Caelo	Miconazole nitrate	2747	1
Caelo	Miconazole nitrate	2773	1
Caelo	Miconazole nitrate	2777	1
Caelo	Miconazole nitrate	2787	1
Caelo	Miconazole nitrate	2796	1
Caelo	Miconazole nitrate	28051306	1
Caelo	Miconazole nitrate	2900/10/14	1
Caelo	Miconazole nitrate	2900/11/15	3
Caelo	Miconazole nitrate	29001614	1
Caelo	Miconazole nitrate	4061304	1
Caelo	Miconazole nitrate	411092-2-P	1
Caelo	Miconazole nitrate	8/AKD4	1
Caelo	Miconazole nitrate	818A-03451	1
Caelo	Miconazole nitrate	8704870	1
Caelo	Miconazole nitrate	8716	1
Caelo	Miconazole nitrate	9177904	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Miconazole nitrate	AKD9	1
Caelo	Miconazole nitrate	F04-3700307	2
Caesar & Lorenz GmbH	Miconazole nitrate	18282113	1
Caesar & Loretz GmbH…	Miconazole nitrate	18282111	1
Caesar & Loretz GmbH…	Miconazole nitrate	18282110	1
Caesar & Loretz GmbH…	Miconazole nitrate	18282113	1
Caesar & Loretz GmbH…	Miconazole nitrate	20000097004	1
Caesar & Loretz GmbH…	Miconazole nitrate	21000827003	1
Caesar & Loretz GmbH…	Miconazole nitrate	21000827017	1
Caesar & Loretz GmbH…	Miconazole nitrate	21000827008	1
Caesar & Loretz GmbH…	Miconazole nitrate	21000827022	2
Caesar & Loretz GmbH…	Miconazole nitrate	21000827003	2
Caesar & Loretz GmbH…	Miconazole nitrate	14149301	1
Caesar & Loretz GmbH…	Miconazole nitrate	11324904	1
Caesar & Loretz GmbH…	Miconazole nitrate	13185602	1
Caesar & Loretz GmbH…	Miconazole nitrate	18282111	2
Caesar & Loretz GmbH…	Miconazole nitrate	18057914	1
Caesar & Loretz GmbH…	Miconazole nitrate	18282106	2
Caesar & Loretz GmbH…	Miconazole nitrate	21000827021	1
Caesar & Loretz GmbH…	Miconazole nitrate	18282105	1
Caesar & Loretz GmbH…	Miconazole nitrate	18282105	1
Caesar & Loretz GmbH…	Miconazole nitrate	2000009703	1
Caesar & Loretz GmbH…	Miconazole nitrate	18282111	1
Caesar & Loretz GmbH/AHD	Miconazole nitrate	20000097003	1
Caesar & Loretz GmbH/AHD	Miconazole nitrate	21000827003	1
Caesar & Loretz GmbH/AHD	Miconazole nitrate	21000827022	1
Caesar & Loretz GmbH…	Miconazole nitrate	18057906	1
Caesar & Loretz GmbH…	Miconazole nitrate	20004304003	2
Caesar & Loretz GmbH/G	Miconazole nitrate	20004304003	1
Caesar & Loretz GmbH/Gehe	Miconazole nitrate	20000097003	1
Caesar & Loretz GmbH/Gehe	Miconazole nitrate	20004304002	1
Caesar & Loretz GmbH/Gehe	Miconazole nitrate	21000827013	1
Caesar & Loretz GmbH/Gehe	Miconazole nitrate	21000827016	1
Caesar & Loretz GmbH…	Miconazole nitrate	20000097007	2
Caesar & Loretz GmbH…	Miconazole nitrate	20000097004	1
Caesar & Loretz GmbH…	Miconazole nitrate	18057913	1
Caesar & Loretz GmbH…	Miconazole nitrate	182821002	1
Caesar & Loretz GmbH…	Miconazole nitrate	18282113	1
Caesar & Loretz GmbH…	Miconazole nitrate	20000097004	2
Caesar & Loretz GmbH…	Miconazole nitrate	20000097009	1
Caesar & Loretz GmbH…	Miconazole nitrate	20004304003	2
Caesar & Loretz GmbH…	Miconazole nitrate	20004304004	1
Caesar & Loretz GmbH…	Miconazole nitrate	21000827001	1
Caesar & Loretz GmbH…	Miconazole nitrate	20004304001	1
Caesar & Loretz GmbH…	Miconazole nitrate	18282113	2
Caesar & Loretz GmbH…	Miconazole nitrate	18282114	1
Caesar & Loretz GmbH…	Miconazole nitrate	21000827014	1
Caesar & Loretz GmbH…	Miconazole nitrate	21000827019	1
Caesar & Loretz GmbH…	Miconazole nitrate		1
Caesar & Loretz GmbH…	Miconazole nitrate	20000097004	1
Caesar & Loretz GmbH…	Miconazole nitrate	20000097007	1
Caesar & Loretz GmbH…	Miconazole nitrate	20004304002	2
Caesar & Loretz GmbH…	Miconazole nitrate	21000827003	1
Caesar & Loretz GmbH/S	Miconazole nitrate	21000827008	2
Caesar & Loretz GmbH…	Miconazole nitrate	18282105	2
Caesar & Loretz GmbH…	Miconazole nitrate	20000097004	1
Caesar & Loretz GmbH…	Miconazole nitrate	20000097005	1
Caesar & Loretz GmbH…	Miconazole nitrate	20004304003	1
Caesar & Loretz GmbH…	Miconazole nitrate	21000827003	2
Caesar & Loretz GmbH…	Miconazole nitrate	18282105	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Miconazole nitrate	16144702	1
Caesar & Loretz GmbH	Miconazole nitrate	16144717	1
Caesar & Loretz GmbH	Miconazole nitrate	18057906	3
Caesar & Loretz GmbH	Miconazole nitrate	18057912	3
Caesar & Loretz GmbH	Miconazole nitrate	18057913	12
Caesar & Loretz GmbH	Miconazole nitrate	18057914	1
Caesar & Loretz GmbH	Miconazole nitrate	18100226	1
Caesar & Loretz GmbH	Miconazole nitrate	182821002	3
Caesar & Loretz GmbH	Miconazole nitrate	18282105	7
Caesar & Loretz GmbH	Miconazole nitrate	18282106	2
Caesar & Loretz GmbH	Miconazole nitrate	18282108	2
Caesar & Loretz GmbH	Miconazole nitrate	18282109	15
Caesar & Loretz GmbH	Miconazole nitrate	18282110	7
Caesar & Loretz GmbH	Miconazole nitrate	18282111	5
Caesar & Loretz GmbH	Miconazole nitrate	18282112	1
Caesar & Loretz GmbH	Miconazole nitrate	18282113	17
Caesar & Loretz GmbH	Miconazole nitrate	18282114	7
Caesar & Loretz GmbH	Miconazole nitrate	19J16-F02	1
Caesar & Loretz GmbH	Miconazole nitrate	20000097002	1
Caesar & Loretz GmbH	Miconazole nitrate	20000097003	8
Caesar & Loretz GmbH	Miconazole nitrate	20000097004	4
Caesar & Loretz GmbH	Miconazole nitrate	20000097005	7
Caesar & Loretz GmbH	Miconazole nitrate	20000097006	4
Caesar & Loretz GmbH	Miconazole nitrate	20000097007	15
Caesar & Loretz GmbH	Miconazole nitrate	20000097009	1
Caesar & Loretz GmbH	Miconazole nitrate	2000097004	1
Caesar & Loretz GmbH	Miconazole nitrate	20004304001	2
Caesar & Loretz GmbH	Miconazole nitrate	20004304002	3
Caesar & Loretz GmbH	Miconazole nitrate	20004304003	9
Caesar & Loretz GmbH	Miconazole nitrate	20004304004	2
Caesar & Loretz GmbH	Miconazole nitrate	21000827001	3
Caesar & Loretz GmbH	Miconazole nitrate	21000827002	9
Caesar & Loretz GmbH	Miconazole nitrate	21000827003	12
Caesar & Loretz GmbH	Miconazole nitrate	21000827006	3
Caesar & Loretz GmbH	Miconazole nitrate	21000827008	5
Caesar & Loretz GmbH	Miconazole nitrate	21000827009	2
Caesar & Loretz GmbH	Miconazole nitrate	21000827010	3
Caesar & Loretz GmbH	Miconazole nitrate	21000827011	4
Caesar & Loretz GmbH	Miconazole nitrate	21000827013	4
Caesar & Loretz GmbH	Miconazole nitrate	21000827014	2
Caesar & Loretz GmbH	Miconazole nitrate	21000827015	4
Caesar & Loretz GmbH	Miconazole nitrate	21000827016	3
Caesar & Loretz GmbH	Miconazole nitrate	21000827017	4
Caesar & Loretz GmbH	Miconazole nitrate	21000827021	2
Caesar & Loretz GmbH	Miconazole nitrate	21000827023	1
Caesar & Loretz GmbH	Miconazole nitrate	F01-3775100	1
Caesar & Loretz Hilden	Miconazole nitrate	18057912	1
Caesar & Loretz Hilden	Miconazole nitrate	18057913	1
Caesar & Loretz Hilden	Miconazole nitrate	18282110	1
Caesar & Loretz Hilden	Miconazole nitrate	18282113	3
Caesar & Loretz Hilden	Miconazole nitrate	20000097003	1
Caesar & Loretz Hilden	Miconazole nitrate	20000097007	1
Caesar & Loretz/AHC	Miconazole nitrate	15137910	1
Caesar & Loretz/Geil...	Miconazole nitrate	20000097003	2
Caesar & Loretz/Geil...	Miconazole nitrate	20000097004	1
Caesar & Loretz/Geil...	Miconazole nitrate	20000097007	1
Caesar & Loretz	Miconazole nitrate	16144724	1
Caesar & Loretz	Miconazole nitrate	18282109	2
Caesar & Loretz	Miconazole nitrate	1850000164	1
Caesar Loretz Gehe	Miconazole nitrate	21000827008	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar und Loretz	Miconazole nitrate	12243805	1
Caesar&Lorenz	Miconazole nitrate	20004304002	1
Caesar&Loretz GmbH ...	Miconazole nitrate	12243808	1
Caesar&Loretz GmbH /Anzag	Miconazole nitrate	14149310	1
Caesar&Loretz GmbH/Anzag	Miconazole nitrate	13185603	1
Caesar&Loretz GmbH/Anzag	Miconazole nitrate	13352802	1
Caesar&loretz,Phoenix	Miconazole nitrate	12374301	1
Cealo / Otto Geilenk...	Miconazole nitrate	18282106	1
Cealo / Otto Geilenk...	Miconazole nitrate	18282111	1
Cealo/Gehe	Miconazole nitrate	20000097007	1
Dr. Wolff	Miconazole nitrate	18E04-B03	1
E+J, 27.09.2016	Miconazole nitrate	15137915	1
Ebert & Jacobi	Miconazole nitrate	15137914	1
Erregierre / Gehe	Miconazole nitrate	18282114	1
Erregierre IT/Noweda	Miconazole nitrate	15137905	1
Erregierre spa	Miconazole nitrate	18282111	1
Erregierre/Noweda	Miconazole nitrate	A180001	1
Erregierre/Noweda	Miconazole nitrate	A190001	1
EuRho/ AHD	Miconazole nitrate	16E04-B03-332373	1
EuRho	Miconazole nitrate	161102401	1
EuRho	Miconazole nitrate	1705039-01	2
euRho	Miconazole nitrate	2009034-01	1
Eurho	Miconazole nitrate	2103012-01	1
euro AHD	Miconazole nitrate	1710020-015633	1
euro AHD	Miconazole nitrate	1710020-015639	1
Euro OTC	Miconazole nitrate	1307025-01	2
Euro OTC	Miconazole nitrate	1307025-02	2
Euro OTC	Miconazole nitrate	140902301	1
Euro OTC	Miconazole nitrate	1409023-01	1
Euro OTC	Miconazole nitrate	140902302	1
Euro OTC	Miconazole nitrate	1409023-02	4
Euro OTC	Miconazole nitrate	1504003-01	2
Euro OTC	Miconazole nitrate	1504903-01	1
Euro OTC	Miconazole nitrate	1509014-01	6
Euro OTC	Miconazole nitrate	1604004-01	5
Euro OTC	Miconazole nitrate	1607004-01	9
Euro OTC	Miconazole nitrate	1611024-01	12
Euro OTC	Miconazole nitrate	1611024-015307	1
Euro OTC	Miconazole nitrate	1611024-015330	1
Euro OTC	Miconazole nitrate	1611024-02	3
Euro OTC	Miconazole nitrate	16144701	1
Euro OTC	Miconazole nitrate	16E04-B03-322124	1
Euro OTC	Miconazole nitrate	16E04-B03-327362	2
Euro OTC	Miconazole nitrate	170503901	1
Euro OTC	Miconazole nitrate	1705039-01	12
Euro OTC	Miconazole nitrate	1705039-015371	1
Euro OTC	Miconazole nitrate	1705039-015432	1
Euro OTC	Miconazole nitrate	1705039-02	6
Euro OTC	Miconazole nitrate	1710020-01	9
Euro OTC	Miconazole nitrate	1710020-015457	1
Euro OTC	Miconazole nitrate	17C01-B02-339699	1
Euro OTC	Miconazole nitrate	17C01-B02-341814	1
Euro OTC	Miconazole nitrate	1803028-01	23
Euro OTC	Miconazole nitrate	18057907	1
Euro OTC	Miconazole nitrate	18057912	1
Euro OTC	Miconazole nitrate	1811015	1
Euro OTC	Miconazole nitrate	181101501	1
Euro OTC	Miconazole nitrate	1811015-01	22
Euro OTC	Miconazole nitrate	1850003395	1
Euro OTC	Miconazole nitrate	19009029-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Miconazole nitrate	1904032-01	1
Euro OTC	Miconazole nitrate	1909029-01	21
Euro OTC	Miconazole nitrate	190929-01	1
Euro OTC	Miconazole nitrate	1950000070	1
Euro OTC	Miconazole nitrate	1950001767	1
Euro OTC	Miconazole nitrate	19A31-B01-359397	1
Euro OTC	Miconazole nitrate	2009034-01	23
Euro OTC	Miconazole nitrate	200903402	1
Euro OTC	Miconazole nitrate	2009034-02	4
Euro OTC	Miconazole nitrate	2009034-03	3
Euro OTC	Miconazole nitrate	20180430/5	1
Euro OTC	Miconazole nitrate	21000827014	1
Euro OTC	Miconazole nitrate	210301201	2
Euro OTC	Miconazole nitrate	2103012-01	19
Euro OTC	Miconazole nitrate	2103012-02	3
Euro OTC	Miconazole nitrate	2103912-02	1
Euro OTC	Miconazole nitrate	2150000385	1
Euro OTC	Miconazole nitrate	22100002-01	1
Euro OTC	Miconazole nitrate	2210002-01	6
Euro OTC	Miconazole nitrate	F02-3670602	1
Euro/Phönix	Miconazole nitrate	1803028-01	3
EuroPTC/Phönix	Miconazole nitrate	14149316	1
Fagron	Miconazole nitrate		1
Fagron	Miconazole nitrate	12/21-M03	1
Fagron	Miconazole nitrate	12A16-N02	2
Fagron	Miconazole nitrate	12H10-N02	4
Fagron	Miconazole nitrate	12K02-N06	5
Fagron	Miconazole nitrate	13061501	1
Fagron	Miconazole nitrate	1316Q-03451	1
Fagron	Miconazole nitrate	1328-N06	1
Fagron	Miconazole nitrate	13A14-B09	2
Fagron	Miconazole nitrate	13A14B09283005	1
Fagron	Miconazole nitrate	13A14-B09-287453	1
Fagron	Miconazole nitrate	13A14-B09-287486	5
Fagron	Miconazole nitrate	13A14-B09-287487	3
Fagron	Miconazole nitrate	13A14-B09-287488	1
Fagron	Miconazole nitrate	13D22-N14	6
Fagron	Miconazole nitrate	13E13-N04	2
Fagron	Miconazole nitrate	13E13-N08	2
Fagron	Miconazole nitrate	13H28_N06	1
Fagron	Miconazole nitrate	13H28-N06	13
Fagron	Miconazole nitrate	13H28-NO6	2
Fagron	Miconazole nitrate	14051403	1
Fagron	Miconazole nitrate	14149313	1
Fagron	Miconazole nitrate	14B18B02	1
Fagron	Miconazole nitrate	14B18-B02	4
Fagron	Miconazole nitrate	14b18-B02-291231	1
Fagron	Miconazole nitrate	14B18-B02-291232	4
Fagron	Miconazole nitrate	14b18-b02-291247	1
Fagron	Miconazole nitrate	14B18-B02-291247	2
Fagron	Miconazole nitrate	14B18-B02-291248	7
Fagron	Miconazole nitrate	14B18-B02-291249	1
Fagron	Miconazole nitrate	14B18-B02-291250	1
Fagron	Miconazole nitrate	14D25-B06	4
Fagron	Miconazole nitrate	14D25-B06-294958	15
Fagron	Miconazole nitrate	14D25-B06-294959	8
Fagron	Miconazole nitrate	14d25-b06-294960	1
Fagron	Miconazole nitrate	14D25-B06-294960	1
Fagron	Miconazole nitrate	14d25-b06-299790	1
Fagron	Miconazole nitrate	14D25-B06-299790	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Miconazole nitrate	14H06-B01-299798	1
Fagron	Miconazole nitrate	14H06-B01-299799	8
Fagron	Miconazole nitrate	14H06-B01-299813	5
Fagron	Miconazole nitrate	14H16-B01-299798	1
Fagron	Miconazole nitrate	15/08-B07-312317	2
Fagron	Miconazole nitrate	15/08-b07-314838	2
Fagron	Miconazole nitrate	15/08-B07-314838	2
Fagron	Miconazole nitrate	15/08-B07-315481	1
Fagron	Miconazole nitrate	15/08-b07-315492	2
Fagron	Miconazole nitrate	15/08-B07-316911	1
Fagron	Miconazole nitrate	15/08-B07-318686	3
Fagron	Miconazole nitrate	15/08-b07-318687	1
Fagron	Miconazole nitrate	1508-B07-314838	1
Fagron	Miconazole nitrate	1508-B07-318686	1
Fagron	Miconazole nitrate	15108-b07-312321	1
Fagron	Miconazole nitrate	15108-B07-318485	1
Fagron	Miconazole nitrate	15137905	1
Fagron	Miconazole nitrate	15137915	1
Fagron	Miconazole nitrate	15A13-807	1
Fagron	Miconazole nitrate	15A13-B07	7
Fagron	Miconazole nitrate	15A13-B07-306565	1
Fagron	Miconazole nitrate	15A13-B07-306791	11
Fagron	Miconazole nitrate	15A13-B07-306791nron	1
Fagron	Miconazole nitrate	15a13-b07-307140	1
Fagron	Miconazole nitrate	15A13-B07-307140	11
Fagron	Miconazole nitrate	15a13-b07-308432	1
Fagron	Miconazole nitrate	15A13-B07-308432	4
Fagron	Miconazole nitrate	15I08-B07	3
Fagron	Miconazole nitrate	15I08-B07-215492	1
Fagron	Miconazole nitrate	15I08-B07-3121321	1
Fagron	Miconazole nitrate	15i08-b07-312317	1
Fagron	Miconazole nitrate	15I08-B07-312317	3
Fagron	Miconazole nitrate	15I08-B07-312321	11
Fagron	Miconazole nitrate	15I08-B07-314838	2
Fagron	Miconazole nitrate	15I08-B07-31485	1
Fagron	Miconazole nitrate	15i08-b07-315481	1
Fagron	Miconazole nitrate	15I08-B07-315481	2
Fagron	Miconazole nitrate	15I08-B07-315492	2
Fagron	Miconazole nitrate	15I08-B07-318485	3
Fagron	Miconazole nitrate	15I08-B07-318686	2
Fagron	Miconazole nitrate	15I08-B07-318687	2
Fagron	Miconazole nitrate	15I18-B07-318485	1
Fagron	Miconazole nitrate	15l08-B07-312321	1
Fagron	Miconazole nitrate	15l08-B07-315492	3
Fagron	Miconazole nitrate	15l08-B07-318686	1
Fagron	Miconazole nitrate	160711M	1
Fagron	Miconazole nitrate	16144702	1
Fagron	Miconazole nitrate	16144703	1
Fagron	Miconazole nitrate	16144725	2
Fagron	Miconazole nitrate	16E04-B03	8
Fagron	Miconazole nitrate	16E04-B03-321354	3
Fagron	Miconazole nitrate	16E04-B03-321367	2
Fagron	Miconazole nitrate	16E04-B03-322124	15
Fagron	Miconazole nitrate	16e04-b03-322131	2
Fagron	Miconazole nitrate	16E04-B03-322131	9
Fagron	Miconazole nitrate	16E04-B03-322132	8
Fagron	Miconazole nitrate	16E04-B03-327362	9
Fagron	Miconazole nitrate	16E04-B03-327367	1
Fagron	Miconazole nitrate	16E04-B03-330082	9
Fagron	Miconazole nitrate	16E04-B03-332373	8

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Miconazole nitrate	17011307	1
Fagron	Miconazole nitrate	17C01B02	1
Fagron	Miconazole nitrate	17C01-B02	6
Fagron	Miconazole nitrate	17C01-B02-225671	1
Fagron	Miconazole nitrate	17c01-b02-334877	1
Fagron	Miconazole nitrate	17C01-B02-334877	8
Fagron	Miconazole nitrate	17C01-B02-334882	4
Fagron	Miconazole nitrate	17c01-b02-335671	1
Fagron	Miconazole nitrate	17C01-B02-335671	6
Fagron	Miconazole nitrate	17C01-B02-338798	3
Fagron	Miconazole nitrate	17c01-b02-340778	1
Fagron	Miconazole nitrate	17C01-B02-340778	15
Fagron	Miconazole nitrate	17C01-B02-341395	4
Fagron	Miconazole nitrate	1811015-01	1
Fagron	Miconazole nitrate	1850000164	4
Fagron	Miconazole nitrate	1850003395	4
Fagron	Miconazole nitrate	18B06-B03	5
Fagron	Miconazole nitrate	18b06-b03-345419	1
Fagron	Miconazole nitrate	18B06-B03-345419	10
Fagron	Miconazole nitrate	18B06-B03-345422	5
Fagron	Miconazole nitrate	18b06-b03-345423	2
Fagron	Miconazole nitrate	18B06-B03-345423	5
Fagron	Miconazole nitrate	18b06-b03-347788	1
Fagron	Miconazole nitrate	18B06-B03-347788	4
Fagron	Miconazole nitrate	18c23-b02	1
Fagron	Miconazole nitrate	18C23-B02	11
Fagron	Miconazole nitrate	18C23-B02-248857	1
Fagron	Miconazole nitrate	18C23-B02-347802	6
Fagron	Miconazole nitrate	18c23-b02-348857	1
Fagron	Miconazole nitrate	18C23-B02-348857	3
Fagron	Miconazole nitrate	18C23-B02-350961	3
Fagron	Miconazole nitrate	18C23-B02-351310	10
Fagron	Miconazole nitrate	18C23-B02-352488	5
Fagron	Miconazole nitrate	18c23-b02-352489	1
Fagron	Miconazole nitrate	18C23-B02-352489	5
Fagron	Miconazole nitrate	18C23-B02-353243	8
Fagron	Miconazole nitrate	18c23-b02-354469	1
Fagron	Miconazole nitrate	18C23-B02-354469	5
Fagron	Miconazole nitrate	18C23-B02-355295	5
Fagron	Miconazole nitrate	18c23-b02-355707	1
Fagron	Miconazole nitrate	18C23-B02-355707	7
Fagron	Miconazole nitrate	18C23-B02-356141	5
Fagron	Miconazole nitrate	18C-B02-354469	1
Fagron	Miconazole nitrate	19041705	1
Fagron	Miconazole nitrate	19051402	1
Fagron	Miconazole nitrate	19500002545P-200709	1
Fagron	Miconazole nitrate	1950002545	6
Fagron	Miconazole nitrate	19A31-B01	11
Fagron	Miconazole nitrate	19A31B0132992	1
Fagron	Miconazole nitrate	19A31-B01-358150	3
Fagron	Miconazole nitrate	19A31-B01-359391	2
Fagron	Miconazole nitrate	19A31-b01-359392	1
Fagron	Miconazole nitrate	19A31-B01-359392	17
Fagron	Miconazole nitrate	19A31B01359396	1
Fagron	Miconazole nitrate	19A31-B01-359396	5
Fagron	Miconazole nitrate	19A31-B01-359397	8
Fagron	Miconazole nitrate	19A31-B01-360612	5
Fagron	Miconazole nitrate	19A31-B01-360613	6
Fagron	Miconazole nitrate	19A31-B01-360614	2
Fagron	Miconazole nitrate	19A31-BO1-359392	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Miconazole nitrate	19F16-F02-366310	1
Fagron	Miconazole nitrate	19J16-F01-367062	1
Fagron	Miconazole nitrate	19J16-F02	7
Fagron	Miconazole nitrate	19J16-F02-366299	1
Fagron	Miconazole nitrate	19J16-F02-366300	8
Fagron	Miconazole nitrate	19J16-F02366310	1
Fagron	Miconazole nitrate	19J16-F02-366310	7
Fagron	Miconazole nitrate	19J16-F02-3663100	1
Fagron	Miconazole nitrate	19J16-F02-366311	14
Fagron	Miconazole nitrate	19J16-F02-3670603	1
Fagron	Miconazole nitrate	19J16-F02-367062	9
Fagron	Miconazole nitrate	19J16-F02-367063	6
Fagron	Miconazole nitrate	19J16-F02-367064	1
Fagron	Miconazole nitrate	19J16-F02-37062	1
Fagron	Miconazole nitrate	20081201	1
Fagron	Miconazole nitrate	2050000157	7
Fagron	Miconazole nitrate	20B21-04-376344	1
Fagron	Miconazole nitrate	20B21-F04	2
Fagron	Miconazole nitrate	20B21-F04-370036	2
Fagron	Miconazole nitrate	20B21-F04-370037	15
Fagron	Miconazole nitrate	20B21-F04-370040	3
Fagron	Miconazole nitrate	20B21-F04-3700400	1
Fagron	Miconazole nitrate	20B21-F04-370270	8
Fagron	Miconazole nitrate	20B21-F04-376344	6
Fagron	Miconazole nitrate	2150000385	3
Fagron	Miconazole nitrate	21C09-F01	5
Fagron	Miconazole nitrate	21C09-F01-277510	1
Fagron	Miconazole nitrate	21C09-F01-37510	1
Fagron	Miconazole nitrate	21C09-F01-37513	1
Fagron	Miconazole nitrate	21C09-F01-377509	1
Fagron	Miconazole nitrate	21C09-F01-377510	11
Fagron	Miconazole nitrate	21C09-F01-377510/215000038	1
Fagron	Miconazole nitrate	21C09-F01-377513	5
Fagron	Miconazole nitrate	22F08_B02_213580	1
Fagron	Miconazole nitrate	22F08-B02	2
Fagron	Miconazole nitrate	22f08-b02-213149	1
Fagron	Miconazole nitrate	22F08-B02-213149	14
Fagron	Miconazole nitrate	22F-08-B02-213149	1
Fagron	Miconazole nitrate	22F08B02213580	1
Fagron	Miconazole nitrate	22F08-B02-221067	5
Fagron	Miconazole nitrate	22F08B02213580	1
Fagron	Miconazole nitrate	2366310	1
Fagron	Miconazole nitrate	27061202	1
Fagron	Miconazole nitrate	2900/03/16	2
Fagron	Miconazole nitrate	2900/04/14	2
Fagron	Miconazole nitrate	2900/08/12	2
Fagron	Miconazole nitrate	2900/09/16	4
Fagron	Miconazole nitrate	2900/10/14	1
Fagron	Miconazole nitrate	2900/11/15	2
Fagron	Miconazole nitrate	2900/15/13	2
Fagron	Miconazole nitrate	2900/16/14	4
Fagron	Miconazole nitrate	2900-03-16	1
Fagron	Miconazole nitrate	29091808	1
Fagron	Miconazole nitrate	20B21-F04-3700400	1
Fagron	Miconazole nitrate	31101306	1
Fagron	Miconazole nitrate	3248	1
Fagron	Miconazole nitrate	4111301	1
Fagron	Miconazole nitrate	8568674	1
Fagron	Miconazole nitrate	B01-3593902	1
Fagron	Miconazole nitrate	B01-3593906	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Miconazole nitrate	B01-359396	1
Fagron	Miconazole nitrate	B01-3606104	1
Fagron	Miconazole nitrate	F01-377510	1
Fagron	Miconazole nitrate	F02-3670602	1
Fagron	Miconazole nitrate	F04-3700307	2
Fagron	Miconazole nitrate	F04-3700400	1
Fagron	Miconazole nitrate	F04-3763404	1
Fargon/Phönix	Miconazole nitrate	19J16-F02-367063	1
Fargon	Miconazole nitrate	14D25-B06-294959	1
Fargon	Miconazole nitrate	18B06-B03-345423	1
Fargon	Miconazole nitrate	22F08-B02-213149	1
Faron	Miconazole nitrate	19A31-B01-359397	1
Fiebig	Miconazole nitrate	15/08-B07-314838	1
Fiebig	Miconazole nitrate	16144726	1
Fischar / Geilenkirchen	Miconazole nitrate	16144726	1
Fragon	Miconazole nitrate	18C23-B02-348857	1
GEHE 13.05	Miconazole nitrate	14149311	1
Gehe 6.03.15	Miconazole nitrate	14149308	2
Gehe am 29.04.2014	Miconazole nitrate	13352802	4
Gehe/Ichthyol	Miconazole nitrate	16E04-B03-322132	1
Gehe	Miconazole nitrate	13352811	1
Gehe	Miconazole nitrate	14149301	1
Gehe	Miconazole nitrate	16144702	1
Gehe	Miconazole nitrate	16144704	1
Gehe	Miconazole nitrate	16144711	1
GEHE	Miconazole nitrate	16144716	1
Gehe	Miconazole nitrate	16144720	1
Gehe	Miconazole nitrate	16E04-B03-327362	1
GEHE	Miconazole nitrate	18057903	1
Gehe	Miconazole nitrate	18282105	1
Gehe	Miconazole nitrate	18B06-B03-345419	1
Gehe	Miconazole nitrate	20000097005	1
Gehe	Miconazole nitrate	21000827003	1
Gehe	Miconazole nitrate	21000827008	2
Gehe	Miconazole nitrate	21000827016	1
Gehe	Miconazole nitrate	21000827023	1
Gehe	Miconazole nitrate	21000827025	2
Gehe	Miconazole nitrate	210301201	1
Gehe	Miconazole nitrate	22F08-B02-221067	3
gehe-06.11.18	Miconazole nitrate	18057906	1
Geibo/Noweda	Miconazole nitrate	17217503	1
Geilenkirchen	Miconazole nitrate	17217505	3
Geilenkirchen	Miconazole nitrate	18057914	1
Hedinger	Miconazole nitrate	16144720	2
Hedinger	Miconazole nitrate	P2018/114	1
Herstellung	Miconazole nitrate	13185602	1
Ichthyol/Phoenix	Miconazole nitrate	16/098/M	1
Jenne	Miconazole nitrate	21000827002	1
Kehr	Miconazole nitrate	17C01-B02-334877	1
Kehr	Miconazole nitrate	21000827022	2
Kehr	Miconazole nitrate	21000827024	3
Kehr	Miconazole nitrate	21000827026	2
Kehr	Miconazole nitrate	22F08-B02	1
Kehr	Miconazole nitrate	23000589004	1
Miconazolnitrat	Miconazole nitrate	20B21-F04-376344	1
Noveda	Miconazole nitrate	18282105	1
Noweda 10.12.2019	Miconazole nitrate	18282106	1
Noweda 26.11.2019	Miconazole nitrate	18282111	1
Noweda	Miconazole nitrate		1
Noweda	Miconazole nitrate	14149310	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Miconazole nitrate	14149311	1
Noweda	Miconazole nitrate	15137903	1
Noweda	Miconazole nitrate	16144704	1
Noweda	Miconazole nitrate	16144721	1
Noweda	Miconazole nitrate	16E04-B03-322124	1
Noweda	Miconazole nitrate	1705039-02	1
Noweda	Miconazole nitrate	17217502	1
Noweda	Miconazole nitrate	17217505	1
Noweda	Miconazole nitrate	18057913	1
Noweda	Miconazole nitrate	18282109	1
Noweda	Miconazole nitrate	18282113	1
Noweda	Miconazole nitrate	19A31-B01-359392	3
Noweda	Miconazole nitrate	20000097003	1
Noweda	Miconazole nitrate	21000827008	1
Noweda	Miconazole nitrate	21000827013	1
Noweda	Miconazole nitrate	21000827022	1
Noweda	Miconazole nitrate	22F08-B02	1
Olon (Lodiagiano)/Sa…	Miconazole nitrate	2050000157	1
Otto Geilenkirchen	Miconazole nitrate	21000827024	1
Phoenix 21.10.14	Miconazole nitrate	14149301	1
Phoenix	Miconazole nitrate	13185611	1
Phoenix	Miconazole nitrate	13352801	1
Phoenix	Miconazole nitrate	15137915	1
Phoenix	Miconazole nitrate	15E04-B03-327367	1
Phoenix	Miconazole nitrate	17C01-B02-334882	1
Phoenix	Miconazole nitrate	18C23-B02-352489	1
Phoenix	Miconazole nitrate	22110002-01	1
Phoenix	Miconazole nitrate	23000589004	1
Phoenix	Miconazole nitrate	B01-3606104	1
PhoenixWE: 28.04.18 …	Miconazole nitrate	17217505	1
Phönix	Miconazole nitrate	13H28-N06	1
phönix	Miconazole nitrate	15137907	1
phönix	Miconazole nitrate	16144701	2
phönix	Miconazole nitrate	16144716	1
Phönix	Miconazole nitrate	16E04-B03-322124	1
Phönix	Miconazole nitrate	16E04-B03-322131	1
Phönix	Miconazole nitrate	17217502	2
Phönix	Miconazole nitrate	18C23-B02-355707	1
Phönix	Miconazole nitrate	1909029-01	1
Phönix	Miconazole nitrate	2009034-01	1
Phönix	Miconazole nitrate	20B21f04376344	1
Phönix	Miconazole nitrate	20B21-F04-376344	1
Phönix	Miconazole nitrate	2103012-01	3
Phönix	Miconazole nitrate	2210002-01	1
Phönix	Miconazole nitrate	3133	1
Sanacop	Miconazole nitrate		1
Sanacorp EK:5,95 …	Miconazole nitrate	16144703	1
Sanacorp W.E:27.03.1…	Miconazole nitrate	16144726	2
Sanacorp	Miconazole nitrate		1
Sanacorp	Miconazole nitrate	12243801	1
Sanacorp	Miconazole nitrate	12243803	2
Sanacorp	Miconazole nitrate	13352801	1
Sanacorp	Miconazole nitrate	16144720	1
Sanacorp	Miconazole nitrate	18057903	1
Sanacorp	Miconazole nitrate	18057912	1
Sanacorp	Miconazole nitrate	18057913	1
Sanacorp	Miconazole nitrate	18282107	1
Sanacorp	Miconazole nitrate	18282108	1
Sanacorp	Miconazole nitrate	18282109	2
Sanacorp	Miconazole nitrate	18282112	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Miconazole nitrate	18282113	1
Sanacorp	Miconazole nitrate	18C23-B02-351310	1
Sanacorp	Miconazole nitrate	21000827006	1
Sanacorp	Miconazole nitrate	21000827008	1
Sanacorp	Miconazole nitrate	21000827011	1
Sanacorp	Miconazole nitrate	21000827015	1
Sanacorp	Miconazole nitrate	21000827023	1
Sanacorp	Miconazole nitrate	21000837088	1
Sanacorp	Miconazole nitrate	2210002-01	1
Sanacorp	Miconazole nitrate	22Fo8-B02-221067	1
Sanacorp	Miconazole nitrate	2900/09/16	1

- 232 811 spectra from 1515 *Apo-Ident* customers from a total of 48 755 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Miconazole nitrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Miconazole nitrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	499	0	152 463
Type B	0	670	0	201 414
Type C	0	3249	7	232 811

The substance/substance group *Miconazole nitrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7976 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.1045 %)
Type C	100.0000 % (> 99.9007 %)	99.7850 % (> 99.6929 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20817	21900	6.37	53.18
20875	21350	8.51	53.35
20905	21900	7.76	46.84
21350	21350	0.00	52.46
21351	21350	2.77	51.09
21649	21900	6.91	51.71
21900	21900	0.00	53.94
22630	22630	0.00	54.91
24593	21900	6.74	53.51

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Minoxidil**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20879-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Minoxidil; Minoxidilum

Special notes

When selecting the *Minoxidil* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Minoxidil	10	20	571

Second-stage model

For differentiation of the substance/substance group *Minoxidil* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Minoxidil* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	70.75	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Minoxidil* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Minoxidil*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Minoxidil	13039501	20879	40	20130306
Caelo	Minoxidil	14093701	21359	40	20140428
Caelo	Minoxidil	14093701	21361	40	20140428
Euro OTC	Minoxidil	1311038-01	21630	59	AR-15-FG-007848-01
Euro OTC	Minoxidil	1411006-01	21912	60	20141210
Euro OTC	Minoxidil	1509035	21933	60	20151016*
Euro OTC	Minoxidil	1602013	22365	60	20160225*
Euro OTC	Minoxidil	1612011	22982	40	20170130*
Euro OTC	Minoxidil	2004030	25162	40	20200528*
Euro OTC	Minoxidil	2109021	25888	50	20211104*
Euro OTC	Minoxidil	2109021	25888SI	50	20211104*
Euro OTC	Minoxidil	2209016	26337	40	20221005*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 579 spectra of 12 reference samples from the substance/substance group *Minoxidil*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 383 spectra from a total of 2832 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1480 spectra of 35 reference samples from the substance/substance group *Minoxidil*.

- Among them are spectra of independent samples from 20 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Minoxidil	172278	23816	40
Caelo	Minoxidil	191957	24758	40
Caelo	Minoxidil	20001705	25613	40
Caelo	Minoxidil	23001171	26845	40
Caelo	Minoxidil	24002249	27436	40
Caelo	Minoxidil	24002248	27441	40
Euro OTC	Minoxidil	1607007	22688	40
Euro OTC	Minoxidil	1705008	23437	40
Euro OTC	Minoxidil	1710043	23896	40
Euro OTC	Minoxidil	1803004	24062	40
Euro OTC	Minoxidil	1807018-01	24190	40
Euro OTC	Minoxidil	1901005	24489	40
Euro OTC	Minoxidil	1907025	24803	40
Euro OTC	Minoxidil	2001035	25120	40
Euro OTC	Minoxidil	2008040	25334	40
Euro OTC	Minoxidil	2008039	25343	40
Euro OTC	Minoxidil	2109018	25866	50
Euro OTC	Minoxidil	2209017	26349	40
Euro OTC	Minoxidil	2311021	27342	40
Fagron	Minoxidil	22C01-B03-218964	26139	40
Caelo	Minoxidil	20001705	25613SI	40
Caelo	Minoxidil	23001171	26845SI	40
Caelo	Minoxidil	24002249	27436SI	40
Caelo	Minoxidil	24002248	27441SI	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Minoxidil	1411006-01	21912SI†	60
Euro OTC	Minoxidil	1509035	21933SI†	60
Euro OTC	Minoxidil	1602013	22365SI†	60
Euro OTC	Minoxidil	1612011	22982SI†	40
Euro OTC	Minoxidil	2008040	25334SI	40
Euro OTC	Minoxidil	2008039	25343SI	40
Euro OTC	Minoxidil	2109018	25866SI	50
Euro OTC	Minoxidil	2209016	26337SI†	40
Euro OTC	Minoxidil	2209017	26349SI	40
Euro OTC	Minoxidil	2311021	27342SI	40
Fagron	Minoxidil	22C01-B03-218964	26139SI	40

- 200 604 spectra from a total of 4020 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3373 spectra from 805 *Apo-Ident* customers from 594 batches from the substance/substance group *Minoxidil*.
- Among them are spectra of independent samples from 541 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Minoxidil	21002063017	1
	Minoxidil	21002063019	1
	Minoxidil	21002063022	4
	Minoxidil	2109018-01	1
	Minoxidil	2109021-01	2
	Minoxidil	2109021-02	5
	Minoxidil	22000546001	3
	Minoxidil	22000546005	1
	Minoxidil	22000546006	3
	Minoxidil	22000546008	4
	Minoxidil	22000546010	6
	Minoxidil	22003	1
	Minoxidil	2209016	1
	Minoxidil	2209016-01	22
	Minoxidil	2209017-01	9
	Minoxidil	2209017-03	1
	Minoxidil	22C01-B03-220935	1
	Minoxidil	22c01-b03-220944	1
	Minoxidil	22I05-B06	1
	Minoxidil	22I05-B06-225227	1
	Minoxidil	22I05-B06-225228	1
	Minoxidil	23001171003	2
	Minoxidil	2300325300	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Minoxidil	23003253001	2
	Minoxidil	23003253003	1
	Minoxidil	23A18-B03-227781	1
	Minoxidil	23D27-B04-230212	1
	Minoxidil	Minox280623	1
/Noweda	Minoxidil	181498002	1
A.H.D	Minoxidil	1210056-01	1
AHC 14.08.13 EK40,14	Minoxidil	1210056-02	1
AHD/Euro	Minoxidil	171004301	1
AHD	Minoxidil	1210056-01	1
AHD	Minoxidil	1311038-01	1
AHD	Minoxidil	1504013-02	1
AHD	Minoxidil	15230812	1
AHD	Minoxidil	18149801	1
AHD	Minoxidil	1907025-02	1
AHD	Minoxidil	200803901	1
AHD	Minoxidil	24B28-B11-236694	1
Alliance health	Minoxidil	1411006-01	3
Alliance Healthc. 15...	Minoxidil	1203035-03	1
Alliance Healthcare	Minoxidil	1210056-01	1
Alliance Healthcare	Minoxidil	1210056-02	1
Alliance Healthcare	Minoxidil	21002063013	1
Alliance	Minoxidil	21002063017	1
Alliance	Minoxidil	2109018-01	1
Alliance	Minoxidil	23A18-B03-227781	1
Anzag 14.11.12 ek:40,14	Minoxidil	120303501	1
Anzag 18.10.12 ek:40,14	Minoxidil	1203035-01	1
Anzag	Minoxidil	1112024-02	1
Anzag	Minoxidil	13E13-N10	1
Anzag	Minoxidil	14234505	1
anzag	Minoxidil	1504013-02	1
api-ident	Minoxidil	1710043-01	2
apo-ident.	Minoxidil	1607007-07	1
Apo-ident	Minoxidil	190102502	1
apomix	Minoxidil	1504013-02	1
apomix	Minoxidil	1602013-01	1
Audor Pharma	Minoxidil		51
Audor Pharma	Minoxidil	20008039-01	1
Audor Pharma	Minoxidil	414E-02844	1
Audor Pharma	Minoxidil	8/14M	1
Audor Pharma	Minoxidil	AP001/16M	7
Audor Pharma	Minoxidil	AP006/13M	2
Audor Pharma	Minoxidil	AP006/17M	5
Audor Pharma	Minoxidil	AP007/15M	4
Audor Pharma	Minoxidil	AP008/14M	6
Audor Pharma	Minoxidil	AP010/12M	5
Audor Pharma	Minoxidil	AP011/16M	2
Audor Pharma	Minoxidil	AP012/16M	4
Audor Pharma	Minoxidil	AP012/16M/5270	1
Audor Pharma	Minoxidil	AP016/15M	8
Audor Pharma	Minoxidil	AP-016/15M	1
Audor Pharma	Minoxidil	AP020/11M	3
Audor Pharma	Minoxidil	AP088/14M	1
Audor Pharma	Minoxidil	APK007	1
Audor Pharma	Minoxidil	APK0071/16/04/065-1M	1
Bombastus	Minoxidil	1112024-03	1
Bombastus	Minoxidil	1705008-01	2
Bombastus	Minoxidil	1710043-01	1
Bombastus	Minoxidil	4/13	1
Caelo	Minoxidil		11

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Minoxidil	1070318/17227803	1
Caelo	Minoxidil	1112024-01	1
Caelo	Minoxidil	11150207	1
Caelo	Minoxidil	11150209	1
Caelo	Minoxidil	11302003	1
Caelo	Minoxidil	11302005	1
Caelo	Minoxidil	11e17-n07	1
Caelo	Minoxidil	11K11-n09	1
Caelo	Minoxidil	12023901	2
Caelo	Minoxidil	12023902	1
Caelo	Minoxidil	12023907	4
Caelo	Minoxidil	12023908	1
Caelo	Minoxidil	1203035	1
Caelo	Minoxidil	1203035-01	1
Caelo	Minoxidil	121005601	1
Caelo	Minoxidil	1210056-01	2
Caelo	Minoxidil	1210056-02	3
Caelo	Minoxidil	12273703	2
Caelo	Minoxidil	12273704	3
Caelo	Minoxidil	12273710	1
Caelo	Minoxidil	12H07-N03	4
Caelo	Minoxidil	13/23-N07	1
Caelo	Minoxidil	13039501	7
Caelo	Minoxidil	13039503	3
Caelo	Minoxidil	130402901	1
Caelo	Minoxidil	130402902	1
Caelo	Minoxidil	1309501	1
Caelo	Minoxidil	1311038-01	2
Caelo	Minoxidil	13179501	2
Caelo	Minoxidil	13179501-3467312121	1
Caelo	Minoxidil	13179502	5
Caelo	Minoxidil	13179503	6
Caelo	Minoxidil	13179504	2
Caelo	Minoxidil	13179507	3
Caelo	Minoxidil	13373106	1
Caelo	Minoxidil	13E13-N10	1
Caelo	Minoxidil	13I23-N07	2
Caelo	Minoxidil	13K04B05290380	1
Caelo	Minoxidil	1405028-01	2
Caelo	Minoxidil	14062018-RQ-A	1
Caelo	Minoxidil	14093702	2
Caelo	Minoxidil	14093703	4
Caelo	Minoxidil	14093706	3
Caelo	Minoxidil	14093707	1
Caelo	Minoxidil	1411006-01	2
Caelo	Minoxidil	14234502	2
Caelo	Minoxidil	14234505	5
Caelo	Minoxidil	14234509	3
Caelo	Minoxidil	14L03-B02-301431	1
Caelo	Minoxidil	150401301	1
Caelo	Minoxidil	1504013-01	5
Caelo	Minoxidil	1504013-02	1
Caelo	Minoxidil	1509035	1
Caelo	Minoxidil	1509035-01	3
Caelo	Minoxidil	1520002455	1
Caelo	Minoxidil	15230802	4
Caelo	Minoxidil	15230803	3
Caelo	Minoxidil	15230804	7
Caelo	Minoxidil	15230805	2
Caelo	Minoxidil	15230806	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Minoxidil	15230811	5
Caelo	Minoxidil	15230812	1
Caelo	Minoxidil	15436024	1
Caelo	Minoxidil	15436201	8
Caelo	Minoxidil	15436202	7
Caelo	Minoxidil	15436202/1060217	1
Caelo	Minoxidil	15436204	3
Caelo	Minoxidil	15436404	4
Caelo	Minoxidil	15436406	5
Caelo	Minoxidil	15436408	8
Caelo	Minoxidil	15436412	2
Caelo	Minoxidil	15436414	6
Caelo	Minoxidil	15436415	2
Caelo	Minoxidil	15E19-B06-308182	1
Caelo	Minoxidil	15E19-B06-308183	1
Caelo	Minoxidil	15E19-B06-309180	1
Caelo	Minoxidil	15H07-B03-317340	1
Caelo	Minoxidil	15K17-B05-318240	1
Caelo	Minoxidil	15K17-B05-318692	1
Caelo	Minoxidil	15K17-B06-321926	1
Caelo	Minoxidil	15k17-b06-324965	1
Caelo	Minoxidil	160013-01	1
Caelo	Minoxidil	1602013-01	9
Caelo	Minoxidil	160201302	2
Caelo	Minoxidil	1602013-02	4
Caelo	Minoxidil	1607007-01	4
Caelo	Minoxidil	160707-01	1
Caelo	Minoxidil	161201101	2
Caelo	Minoxidil	1612011-01	8
Caelo	Minoxidil	16J24-B04-328218	1
Caelo	Minoxidil	16J24-B05-331128	1
Caelo	Minoxidil	16J24-B05-332092	1
Caelo	Minoxidil	170043-01	1
Caelo	Minoxidil	17011602	1
Caelo	Minoxidil	170500801	5
Caelo	Minoxidil	1705008-01	7
Caelo	Minoxidil	1710043-01	8
Caelo	Minoxidil	17227801	18
Caelo	Minoxidil	17227803	20
Caelo	Minoxidil	17228703	1
Caelo	Minoxidil	17H08-B06-341377	1
Caelo	Minoxidil	17H08-B06-342282	1
Caelo	Minoxidil	18016103	2
Caelo	Minoxidil	18016104	3
Caelo	Minoxidil	18016107	5
Caelo	Minoxidil	18016109	8
Caelo	Minoxidil	18016112	2
Caelo	Minoxidil	1803004-001	1
Caelo	Minoxidil	1803004-01	3
Caelo	Minoxidil	1807018_01	1
Caelo	Minoxidil	180701801	1
Caelo	Minoxidil	1807018-01	8
Caelo	Minoxidil	181498001	1
Caelo	Minoxidil	181498002	2
Caelo	Minoxidil	18149801	7
Caelo	Minoxidil	18149802	18
Caelo	Minoxidil	18149805	4
Caelo	Minoxidil	18149810	7
Caelo	Minoxidil	18149811	1
Caelo	Minoxidil	18149813	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Minoxidil	18149815	17
Caelo	Minoxidil	18159810	1
Caelo	Minoxidil	187018-01	1
Caelo	Minoxidil	18C20-B01-35661844	1
Caelo	Minoxidil	18C27-B01	1
Caelo	Minoxidil	1901005-01	3
Caelo	Minoxidil	190702501	1
Caelo	Minoxidil	1907025-01	1
Caelo	Minoxidil	190702502	1
Caelo	Minoxidil	19149810	1
Caelo	Minoxidil	19157002	1
Caelo	Minoxidil	191957002	7
Caelo	Minoxidil	191957003	7
Caelo	Minoxidil	191957004	5
Caelo	Minoxidil	191957007	7
Caelo	Minoxidil	191957010	6
Caelo	Minoxidil	200001705004	1
Caelo	Minoxidil	2000040	1
Caelo	Minoxidil	20001705004	4
Caelo	Minoxidil	20004048001	2
Caelo	Minoxidil	20004048003	9
Caelo	Minoxidil	20004048005	5
Caelo	Minoxidil	20004048008	2
Caelo	Minoxidil	20004048009	7
Caelo	Minoxidil	20004048012	2
Caelo	Minoxidil	2000408012	1
Caelo	Minoxidil	200804001	1
Caelo	Minoxidil	2008040-01	1
Caelo	Minoxidil	20151112-5	1
Caelo	Minoxidil	20160211-1	1
Caelo	Minoxidil	21002063001	9
Caelo	Minoxidil	21002063003	8
Caelo	Minoxidil	21002063005	2
Caelo	Minoxidil	21002063006	8
Caelo	Minoxidil	21002063009	2
Caelo	Minoxidil	21002063011	4
Caelo	Minoxidil	21002063012	3
Caelo	Minoxidil	21002063013	4
Caelo	Minoxidil	21002063015	2
Caelo	Minoxidil	21002063017	4
Caelo	Minoxidil	21002063018	12
Caelo	Minoxidil	210902101	1
Caelo	Minoxidil	22000546005	2
Caelo	Minoxidil	22000546008	2
Caelo	Minoxidil	22031402	1
Caelo	Minoxidil	2827	1
Caelo	Minoxidil	2905047-01	1
Caelo	Minoxidil	3013M-02844	1
Caelo	Minoxidil	31051305	1
Caelo	Minoxidil	41/17	1
Caelo	Minoxidil	5081502	1
Caelo	Minoxidil	5217M-02844	1
Caelo	Minoxidil	8719	1
Caelo	Minoxidil	AP006/17M	1
Caelo	Minoxidil	AP011/16M	1
Caelo	Minoxidil	K0071/16/04/065	1
Caesaer/Jenne	Minoxidil	18016103	1
Caesar & Loretz GmbH...	Minoxidil	14093702	1
Caesar & Loretz GmbH...	Minoxidil	14234505	1
Caesar & Loretz GmbH...	Minoxidil	18149813	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/AHD	Minoxidil	20004048009	1
Caesar & Loretz GmbH...	Minoxidil	20004048005	1
Caesar & Loretz GmbH...	Minoxidil	20004048008	1
Caesar & Loretz GmbH...	Minoxidil	191957002	1
Caesar & Loretz GmbH...	Minoxidil	20004048012	1
Caesar & Loretz GmbH...	Minoxidil	21002063006	3
Caesar & Loretz GmbH...	Minoxidil	21002063004	3
Caesar & Loretz GmbH	Minoxidil		1
Caesar & Loretz GmbH	Minoxidil	13039501	1
Caesar & Loretz GmbH	Minoxidil	17227803	1
Caesar & Loretz GmbH	Minoxidil	181498002	1
Caesar & Loretz GmbH	Minoxidil	18149801	1
Caesar & Loretz GmbH	Minoxidil	18149802	6
Caesar & Loretz GmbH	Minoxidil	18149810	2
Caesar & Loretz GmbH	Minoxidil	18149813	3
Caesar & Loretz GmbH	Minoxidil	18149815	5
Caesar & Loretz GmbH	Minoxidil	191957002	4
Caesar & Loretz GmbH	Minoxidil	191957004	3
Caesar & Loretz GmbH	Minoxidil	191957007	5
Caesar & Loretz GmbH	Minoxidil	191957010	3
Caesar & Loretz GmbH	Minoxidil	20001705004	7
Caesar & Loretz GmbH	Minoxidil	20004048003	2
Caesar & Loretz GmbH	Minoxidil	20004048005	7
Caesar & Loretz GmbH	Minoxidil	20004048008	4
Caesar & Loretz GmbH	Minoxidil	20004048009	3
Caesar & Loretz GmbH	Minoxidil	20004048012	1
Caesar & Loretz GmbH	Minoxidil	21000123003	1
Caesar & Loretz GmbH	Minoxidil	21002063001	3
Caesar & Loretz GmbH	Minoxidil	21002063003	2
Caesar & Loretz GmbH	Minoxidil	21002063004	1
Caesar & Loretz GmbH	Minoxidil	21002063005	2
Caesar & Loretz GmbH	Minoxidil	21002063006	2
Caesar & Loretz GmbH	Minoxidil	21002063011	2
Caesar & Loretz GmbH	Minoxidil	21002063012	3
Caesar & Loretz GmbH	Minoxidil	21002063017	1
Caesar & Loretz GmbH	Minoxidil	21002063018	1
Caesar & Loretz GmbH	Minoxidil	22000546001	1
Caesar & Loretz GmbH	Minoxidil	22000546005	1
Caesar & Loretz GmbH	Minoxidil	22000546008	1
Caesar & Loretz	Minoxidil	15436414	1
Caleo/ Noweda	Minoxidil	18016104	1
Doppeleiche Apotheke	Minoxidil	13E13-N10	2
Dr. Wolff / Sanacorp	Minoxidil	1901005-01	2
EuRho / 2	Minoxidil	2004030-01	1
EuRho / AHD 19.08.21...	Minoxidil	2008040-01	2
EuRho / Noweda	Minoxidil	1304029-02	1
EuRho / Sanacorp	Minoxidil	1710043-01	1
EuRho /Sanacorp	Minoxidil	2008040-01	2
EuRho/ Alliance	Minoxidil	1705008-01	1
EuRho/ Alliance	Minoxidil	1901005-01	1
EuRho/ Noweda	Minoxidil	1807018-01	1
EuRho/ NOWEDA	Minoxidil	1807018-01	1
EuRho/ Phoenix	Minoxidil	2109018-01	2
EuRho/Anzag	Minoxidil	1411006-01	1
EuRho/Fiebig	Minoxidil	1411006-01	1
EuRho/Gehe	Minoxidil	2008039-01	2
EuRho/Gehe	Minoxidil	2109018-01	1
EuRho/Kehr	Minoxidil	1803004-01	2
EuRho/Kehr	Minoxidil	30/17	1
EuRho/Noweda	Minoxidil	1607007-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho/Noweda	Minoxidil	1710043-01	2
Eurho/Phönix	Minoxidil	2004030-01	1
Eurho/Phönix	Minoxidil	2008039-01	1
EuRho/Sanacorp	Minoxidil	17050008-01	1
EuRho/Sanacorp	Minoxidil	1803004-01	2
EuRho/Sanacorp	Minoxidil	1901005-01	1
EuRho/Sanacorp	Minoxidil	1907025-01	2
EuRho/Sanacorp	Minoxidil	2004030-01	1
EuRho	Minoxidil	1105030-02	1
EuRho	Minoxidil	1108039-02	2
EuRho	Minoxidil	1602013-02	1
eurho	Minoxidil	1705008-01	1
EuRho	Minoxidil	1705008-01	1
EuRho	Minoxidil	1710043-01	3
Eurho	Minoxidil	1803004-01	2
EuRho	Minoxidil	1803004-01	1
EuRho	Minoxidil	1901005-01	3
EuRho	Minoxidil	2004030-01	5
EuRho	Minoxidil	2008039-01	2
euRho	Minoxidil	2008040-01	1
EuRho	Minoxidil	2008040-01	1
EuRho	Minoxidil	2109018-01	2
Eurho	Minoxidil	2109021-02	2
Euro OCT / Krieger	Minoxidil	2001035-01	1
Euro OT/Phönix	Minoxidil	1710043-01	1
Euro OTC	Minoxidil		17
Euro OTC	Minoxidil	/18/07/1402	1
Euro OTC	Minoxidil	10/13	1
Euro OTC	Minoxidil	1009042-01	3
Euro OTC	Minoxidil	103004-01	1
Euro OTC	Minoxidil	104029-02	1
Euro OTC	Minoxidil	1102010-02	1
Euro OTC	Minoxidil	1108039-01	1
Euro OTC	Minoxidil	1108039-03	1
Euro OTC	Minoxidil	1112024-01	1
Euro OTC	Minoxidil	1112024-02	5
Euro OTC	Minoxidil	1112024-03	3
Euro OTC	Minoxidil	12/16	2
Euro OTC	Minoxidil	12/17	2
Euro OTC	Minoxidil	1203035	1
Euro OTC	Minoxidil	1203035-01	10
Euro OTC	Minoxidil	1203035-02	6
Euro OTC	Minoxidil	120303503	1
Euro OTC	Minoxidil	1203035-03	11
Euro OTC	Minoxidil	12100056-01	1
Euro OTC	Minoxidil	121005601	1
Euro OTC	Minoxidil	1210056-01	14
Euro OTC	Minoxidil	1210056-02	26
Euro OTC	Minoxidil	13001	1
Euro OTC	Minoxidil	130402901	1
Euro OTC	Minoxidil	1304029-01	16
Euro OTC	Minoxidil	130402902	1
Euro OTC	Minoxidil	1304029-02	15
Euro OTC	Minoxidil	1304029-C2	1
Euro OTC	Minoxidil	131103801	4
Euro OTC	Minoxidil	1311038-01	30
Euro OTC	Minoxidil	13110838-01	1
Euro OTC	Minoxidil	140502801	3
Euro OTC	Minoxidil	1405028-01	29
Euro OTC	Minoxidil	14050281	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Minoxidil	1405028-1	1
Euro OTC	Minoxidil	140528-01	1
Euro OTC	Minoxidil	141100601	5
Euro OTC	Minoxidil	1411006-01	43
Euro OTC	Minoxidil	1411006601	1
Euro OTC	Minoxidil	150401-01	1
Euro OTC	Minoxidil	1504013-01	36
Euro OTC	Minoxidil	1504013-02	27
Euro OTC	Minoxidil	1504013-2	1
Euro OTC	Minoxidil	15081829	1
Euro OTC	Minoxidil	1509035-01	42
Euro OTC	Minoxidil	15436404	1
Euro OTC	Minoxidil	160201301	1
Euro OTC	Minoxidil	1602013-01	44
Euro OTC	Minoxidil	1602013-02	14
Euro OTC	Minoxidil	1602013-1	1
Euro OTC	Minoxidil	1602016-01	1
Euro OTC	Minoxidil	16070007-01	1
Euro OTC	Minoxidil	1607001-01	1
Euro OTC	Minoxidil	1607007	1
Euro OTC	Minoxidil	160700701	3
Euro OTC	Minoxidil	1607007-01	40
Euro OTC	Minoxidil	16112011-01	2
Euro OTC	Minoxidil	16120-01	1
Euro OTC	Minoxidil	161201-01	1
Euro OTC	Minoxidil	1612011	1
Euro OTC	Minoxidil	161201101	2
Euro OTC	Minoxidil	1612011-01	81
Euro OTC	Minoxidil	1612011-011	1
Euro OTC	Minoxidil	16122011_01	1
Euro OTC	Minoxidil	17050008	1
Euro OTC	Minoxidil	1705008_01	1
Euro OTC	Minoxidil	170500801	3
Euro OTC	Minoxidil	1705008-01	57
Euro OTC	Minoxidil	1707018-01	1
Euro OTC	Minoxidil	170703M/1602013-02	1
Euro OTC	Minoxidil	1710043_01	1
Euro OTC	Minoxidil	171004301	9
Euro OTC	Minoxidil	1710043-01	103
Euro OTC	Minoxidil	17100-43-01	1
Euro OTC	Minoxidil	1710043-03	1
Euro OTC	Minoxidil	17H08-B06	1
Euro OTC	Minoxidil	17H08-B06-342282	1
Euro OTC	Minoxidil	17H08-B09-346945	1
Euro OTC	Minoxidil	18030004-01	1
Euro OTC	Minoxidil	1803004	1
Euro OTC	Minoxidil	1803004_01	2
Euro OTC	Minoxidil	180300401	7
Euro OTC	Minoxidil	1803004-01	115
Euro OTC	Minoxidil	180304-01	1
Euro OTC	Minoxidil	1807017-01	1
Euro OTC	Minoxidil	1807018	1
Euro OTC	Minoxidil	180701801	1
Euro OTC	Minoxidil	1807018-01	60
Euro OTC	Minoxidil	1807018-02	3
Euro OTC	Minoxidil	180708-01	1
Euro OTC	Minoxidil	180718-01	1
Euro OTC	Minoxidil	19/15	1
Euro OTC	Minoxidil	19/16	1
Euro OTC	Minoxidil	190100-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Minoxidil	19010005-01	1
Euro OTC	Minoxidil	190100501	3
Euro OTC	Minoxidil	1901005-01	83
Euro OTC	Minoxidil	19011005-01	1
Euro OTC	Minoxidil	1907025	1
Euro OTC	Minoxidil	1907025_01	1
Euro OTC	Minoxidil	190702501	4
Euro OTC	Minoxidil	1907025-01	63
Euro OTC	Minoxidil	190702502	4
Euro OTC	Minoxidil	1907025-02	38
Euro OTC	Minoxidil	1907025-41	1
Euro OTC	Minoxidil	1919	1
Euro OTC	Minoxidil	20004048005	1
Euro OTC	Minoxidil	2000804001	1
Euro OTC	Minoxidil	20008040-01	1
Euro OTC	Minoxidil	2001035-01	23
Euro OTC	Minoxidil	2002312844	1
Euro OTC	Minoxidil	2004020-01	1
Euro OTC	Minoxidil	200403001	9
Euro OTC	Minoxidil	2004030-01	119
Euro OTC	Minoxidil	2004030-1	2
Euro OTC	Minoxidil	20080039-01	1
Euro OTC	Minoxidil	200803901	9
Euro OTC	Minoxidil	2008039-01	95
Euro OTC	Minoxidil	2008040	2
Euro OTC	Minoxidil	2008040_01	2
Euro OTC	Minoxidil	200804001	2
Euro OTC	Minoxidil	2008040-01	108
Euro OTC	Minoxidil	2008040-1	1
Euro OTC	Minoxidil	200840-01	1
Euro OTC	Minoxidil	2091714	1
Euro OTC	Minoxidil	210018-01	1
Euro OTC	Minoxidil	2103021-02	1
Euro OTC	Minoxidil	2109018	1
Euro OTC	Minoxidil	210901801	2
Euro OTC	Minoxidil	2109018-01	69
Euro OTC	Minoxidil	2109021-01	23
Euro OTC	Minoxidil	2109021-02	12
Euro OTC	Minoxidil	210918-01	1
Euro OTC	Minoxidil	210921-02	1
Euro OTC	Minoxidil	2209016-01	4
Euro OTC	Minoxidil	29071402	1
Euro OTC	Minoxidil	4/13	2
Euro OTC	Minoxidil	4004030-01	1
Euro OTC	Minoxidil	6/12	2
Euro OTC	Minoxidil	6614849	1
Euro OTC	Minoxidil	700158	1
Euro Pharm/Gehe	Minoxidil	1901005-01	1
euro pharm	Minoxidil	1590035	1
Euro/ Phönix	Minoxidil	1405028-01	1
EUro/AHD	Minoxidil	1203035-03	2
Euro/Anzag	Minoxidil	150903501	1
Euro/Gehe	Minoxidil	1112024-03	1
Euro/Gehe	Minoxidil	140528-01	1
Euro/Krieger	Minoxidil	1602013-02	1
Euro/Noweda	Minoxidil	1602013-02	1
Euro/Noweda	Minoxidil	1612011-01	1
Euro/Phönix	Minoxidil	161201101	2
Euro/Phönix	Minoxidil	1612011-01	1
Euro/Phönix	Minoxidil	1901005	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro/Phönix	Minoxidil	1901005-01	3
Euro/Phönix	Minoxidil	2001035-01	1
Euro/Phönix	Minoxidil	20044030-01	1
Euro/Phönix	Minoxidil	210901801	2
Euro	Minoxidil	1304029-02	1
Euro	Minoxidil	1504013-01	2
euro	Minoxidil	2008039-01	1
euroct/Gehe	Minoxidil	1304029-01	1
EuRoh/ Gehe	Minoxidil	2008039-01	1
EuRoh	Minoxidil	2008040-01	1
europharm/gehe	Minoxidil	1710043-01	1
Europharm/Sanacorp	Minoxidil	1210056-01	1
EurPS	Minoxidil	1504013-01	2
Faagron/Fiebig 09.04.19	Minoxidil	18c27-B01-354525	1
Fagrin	Minoxidil	15K17-B06-321926	1
Fagron	Minoxidil		2
Fagron	Minoxidil	1/16M	2
Fagron	Minoxidil	11021402	1
Fagron	Minoxidil	11E17-N07	1
Fagron	Minoxidil	11H07-N03	1
Fagron	Minoxidil	11K11-N09	2
Fagron	Minoxidil	120303503	1
Fagron	Minoxidil	1210056-02	1
Fagron	Minoxidil	12A25-N04	4
Fagron	Minoxidil	12C29-N05	4
Fagron	Minoxidil	12C29-N050087/240	1
Fagron	Minoxidil	12C29-N050145/240	1
Fagron	Minoxidil	12H07N03	1
Fagron	Minoxidil	12H07-N03	12
Fagron	Minoxidil	12H07-N030265/432	1
Fagron	Minoxidil	12H07-No3	1
Fagron	Minoxidil	12H07-NO3	1
Fagron	Minoxidil	12HO7-NO3	1
Fagron	Minoxidil	1311038-01	2
Fagron	Minoxidil	13E13N10	1
Fagron	Minoxidil	13E13-N10	9
Fagron	Minoxidil	13H07-NO3	1
Fagron	Minoxidil	13I23-N07	8
Fagron	Minoxidil	13J23N07	2
Fagron	Minoxidil	13J29-B02	1
Fagron	Minoxidil	13K04-B05-0004	1
Fagron	Minoxidil	13K04-B05-290377	6
Fagron	Minoxidil	13K04-B05-290379	2
Fagron	Minoxidil	13K04-B05-290380	3
Fagron	Minoxidil	13123-N07	1
Fagron	Minoxidil	1411006-01	2
Fagron	Minoxidil	1420001962	1
Fagron	Minoxidil	14B04-B07	1
Fagron	Minoxidil	14B04-B07-290883	3
Fagron	Minoxidil	14B04-B07-297364	1
Fagron	Minoxidil	14L03-B02	3
Fagron	Minoxidil	14L03-B02-30129	1
Fagron	Minoxidil	14L03-B02-301428	1
Fagron	Minoxidil	14L03-B02301429	1
Fagron	Minoxidil	14L03-B02-301429	7
Fagron	Minoxidil	14L03-B02-301430	2
Fagron	Minoxidil	14L03-B02-301431	1
Fagron	Minoxidil	14L03-B02301434	1
Fagron	Minoxidil	14L03-B02-301541	1
Fagron	Minoxidil	14L03-Bo2-301430	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Minoxidil	1504013-01	2
Fagron	Minoxidil	1510001251	3
Fagron	Minoxidil	1520000768	2
Fagron	Minoxidil	1520002631	2
Fagron	Minoxidil	15436408	1
Fagron	Minoxidil	15E19-06-308183	1
Fagron	Minoxidil	15E19-B06	1
Fagron	Minoxidil	15E19-B06-308179	1
Fagron	Minoxidil	15e19-b06-308180	1
Fagron	Minoxidil	15E19-B06-308180	5
Fagron	Minoxidil	15E19-B06-308181	6
Fagron	Minoxidil	15E19-B06-308182	5
Fagron	Minoxidil	15E19-B06-308183	6
Fagron	Minoxidil	15E19-B09-308181	1
Fagron	Minoxidil	15E19-B06-308183	1
Fagron	Minoxidil	15F02-B08	1
Fagron	Minoxidil	15F02-B09-312663	2
Fagron	Minoxidil	15H07-B01-313607	1
Fagron	Minoxidil	15H07-B01-314726	2
Fagron	Minoxidil	15K17-B05	1
Fagron	Minoxidil	15K17-B05-318240	2
Fagron	Minoxidil	15K17-B05-318241	2
Fagron	Minoxidil	15K17-B05-318411	2
Fagron	Minoxidil	15K17-B05-318691	4
Fagron	Minoxidil	15K17-B05-318692	1
Fagron	Minoxidil	15K17-B05-320188	3
Fagron	Minoxidil	15K17-B06	1
Fagron	Minoxidil	15K17-B06-321926	5
Fagron	Minoxidil	15K17-B06-321927	3
Fagron	Minoxidil	15K17-B06-321928	2
Fagron	Minoxidil	15k17-b06-324965	1
Fagron	Minoxidil	15K17-B06-324965	3
Fagron	Minoxidil	15K17-B06-325490	3
Fagron	Minoxidil	15K17-B06-325491	2
Fagron	Minoxidil	15K197-B05-318411	1
Fagron	Minoxidil	16/24-B04-328218	1
Fagron	Minoxidil	1612011-01	1
Fagron	Minoxidil	16j24-b04328218	1
Fagron	Minoxidil	16J24-B04-328218	6
Fagron	Minoxidil	16J24-B04-328219	1
Fagron	Minoxidil	16J24-B04-328224	2
Fagron	Minoxidil	16J24-B04-328225	1
Fagron	Minoxidil	16J24-B04-328226	3
Fagron	Minoxidil	16j24-B04-329291	1
Fagron	Minoxidil	16J24-B04-329291	1
Fagron	Minoxidil	16J24-B05	1
Fagron	Minoxidil	16J24-B05-332092	5
Fagron	Minoxidil	16J24-B05-332093	2
Fagron	Minoxidil	1705008-01	2
Fagron	Minoxidil	170612184	1
Fagron	Minoxidil	1722	1
Fagron	Minoxidil	17B22/B02/336689	2
Fagron	Minoxidil	17b22-b01	1
Fagron	Minoxidil	17B22-B01	2
Fagron	Minoxidil	17B22-B01-334447	1
Fagron	Minoxidil	17B22-B01-335427	8
Fagron	Minoxidil	17B22-B02	2
Fagron	Minoxidil	17B22-B02-336689	3
Fagron	Minoxidil	17B22-B02-336690	1
Fagron	Minoxidil	17B22-B02-336700	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Minoxidil	17B22-B02-338766	3
Fagron	Minoxidil	17B22-B02-338767	1
Fagron	Minoxidil	17H08-B06	1
Fagron	Minoxidil	17H08-B06-340512	2
Fagron	Minoxidil	17H08-B06-340514	2
Fagron	Minoxidil	17H08-B06-341376	5
Fagron	Minoxidil	17H08-B06-341377	5
Fagron	Minoxidil	17h08-b06-342282	1
Fagron	Minoxidil	17H08-B09	4
Fagron	Minoxidil	17H08-B09-346945	3
Fagron	Minoxidil	17H08-B09-346947	2
Fagron	Minoxidil	17H08-B09-346948	1
Fagron	Minoxidil	17H08-B09-347482	1
Fagron	Minoxidil	18002	2
Fagron	Minoxidil	18003	1
Fagron	Minoxidil	18004	3
Fagron	Minoxidil	18008	4
Fagron	Minoxidil	1803004-01	2
Fagron	Minoxidil	18C19-B01-348984	4
Fagron	Minoxidil	18C19-B01-348985	2
Fagron	Minoxidil	18C20-B01	4
Fagron	Minoxidil	18C20-b01-351844	1
Fagron	Minoxidil	18C20-B01-351844	4
Fagron	Minoxidil	18C20-B01-352113	1
Fagron	Minoxidil	18C20-B01-352116	2
Fagron	Minoxidil	18C20-B01-352629	5
Fagron	Minoxidil	18C20-B01-352702	5
Fagron	Minoxidil	18C20-B01-352874	1
Fagron	Minoxidil	18C27-B01-354524	3
Fagron	Minoxidil	18C27-B01-354525	7
Fagron	Minoxidil	18C27-B01-354782	1
Fagron	Minoxidil	18C-B01-352116	1
Fagron	Minoxidil	18L19-B05-356595	6
Fagron	Minoxidil	18L19-BO5-356595	1
Fagron	Minoxidil	19002	2
Fagron	Minoxidil	19003	5
Fagron	Minoxidil	19004	1
Fagron	Minoxidil	1901005-01	1
Fagron	Minoxidil	1907025-01	2
Fagron	Minoxidil	19b18-b06-191023	1
Fagron	Minoxidil	19B21-190615	1
Fagron	Minoxidil	19B21-B07	1
Fagron	Minoxidil	19B21-B07-190615	9
Fagron	Minoxidil	19B21-B07-190616	2
Fagron	Minoxidil	19B21-B07-190617	6
Fagron	Minoxidil	19B21-B07-190618	9
Fagron	Minoxidil	19B21-B07-190628	1
Fagron	Minoxidil	19B21-B07-190661	1
Fagron	Minoxidil	19B21-B07-19618	1
Fagron	Minoxidil	19E28-B12	3
Fagron	Minoxidil	19E28-B12_193438	1
Fagron	Minoxidil	19E28-B12-1934308	1
Fagron	Minoxidil	19E28-B12-193438	9
Fagron	Minoxidil	19E28-B12-193440	1
Fagron	Minoxidil	19E28-B12-193447	1
Fagron	Minoxidil	19E28-B12-193449	4
Fagron	Minoxidil	19g22-B02	1
Fagron	Minoxidil	19G22-B02	2
Fagron	Minoxidil	19G22-B02-193448	10
Fagron	Minoxidil	19G22-B02-1934939	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Minoxidil	19G22-B02-193448	1
Fagron	Minoxidil	2/16M	4
Fagron	Minoxidil	2008039-01	1
Fagron	Minoxidil	20A07-B02-197710	1
Fagron	Minoxidil	20A07-b02-197718	1
Fagron	Minoxidil	20A07-B02-197718	1
Fagron	Minoxidil	20A07-B02-197719	2
Fagron	Minoxidil	20A07-B02-197720	3
Fagron	Minoxidil	20A15-B99	1
Fagron	Minoxidil	20A15-B99_196663	1
Fagron	Minoxidil	20A15-B99-196663	8
Fagron	Minoxidil	20A15-B99-196664	1
Fagron	Minoxidil	20A15-B99-196667	2
Fagron	Minoxidil	20A15-B99-196668	1
Fagron	Minoxidil	20D27-B11	1
Fagron	Minoxidil	20D27-B11-201184	3
Fagron	Minoxidil	20D27-B11-201247	2
Fagron	Minoxidil	20D27-B11-201331	2
Fagron	Minoxidil	20K05-B03-202207	2
Fagron	Minoxidil	21001	1
Fagron	Minoxidil	21B02-B13	2
Fagron	Minoxidil	21B02-B13-2153704	1
Fagron	Minoxidil	21B02-B13-215374	2
Fagron	Minoxidil	21B11_B18_203082	1
Fagron	Minoxidil	21B11-B18	1
Fagron	Minoxidil	21B11-B18-203081	3
Fagron	Minoxidil	21B11-B18-203082	1
Fagron	Minoxidil	21B11-B18-203084	2
Fagron	Minoxidil	21B11-B20-210128	6
Fagron	Minoxidil	21B16-B15-220936	1
Fagron	Minoxidil	21B16B15220943	1
Fagron	Minoxidil	21F07-B05-215378	5
Fagron	Minoxidil	21F07-B06	1
Fagron	Minoxidil	21F07-B06-213152	1
Fagron	Minoxidil	21F07-B07-0004	1
Fagron	Minoxidil	21F07-B07-216774	4
Fagron	Minoxidil	21F07-B07-216859	2
Fagron	Minoxidil	21F07-B07-216892	1
Fagron	Minoxidil	21F07-B07-216984	1
Fagron	Minoxidil	21J06-B05-213146	3
Fagron	Minoxidil	21JO6-B05-213146	1
Fagron	Minoxidil	22C01_b03-21915	1
Fagron	Minoxidil	22C01-B03	1
Fagron	Minoxidil	22C01-B03-218964	4
Fagron	Minoxidil	22C01-B03-220935	1
Fagron	Minoxidil	26111302	1
Fagron	Minoxidil	27081301	1
Fagron	Minoxidil	2OD27-B11-201218	1
Fagron	Minoxidil	321926	1
Fagron	Minoxidil	4110I-02844	1
Fagron	Minoxidil	5/17M	1
Fagron	Minoxidil	612212844	1
Fagron	Minoxidil	7/13	1
Fagron	Minoxidil	B02-1934309	1
Fagron	Minoxidil	B05-215378	2
Fagron	Minoxidil	B11-2011804	1
Fagron	Minoxidil	B12-1934409	1
Fagron	Minoxidil	B13-2131407	1
Fagron	Minoxidil	B18-2030801	2
Fagron	Minoxidil	B99-1966607	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fargon	Minoxidil	20A15-B97-197717	1
Fargon	Minoxidil	21B11-B20-210128	1
Fiebig ek: 36.06EUR 31.0812	Minoxidil	111202403	1
Fiebig	Minoxidil	1509035-01	1
Fiebig	Minoxidil	1607007-01	1
Fiebig	Minoxidil	1612011-01	1
Fiebig	Minoxidil	1705008-01	1
Fiebig	Minoxidil	171004301	1
Fiebig	Minoxidil	1710043-01	1
Fiebig	Minoxidil	1807017-01	1
Fiebig	Minoxidil	1901005-01	1
Fiebig	Minoxidil	1907025	1
Fiebig	Minoxidil	1907025-02	1
Fiebig	Minoxidil	2004030-01	1
Fragon	Minoxidil	20K05-B03-202207	1
Gatt-Koller	Minoxidil	1803103	2
Gehe / EuRho	Minoxidil	1803004-01	1
GEHE 07.05.2014	Minoxidil	1311038-01	2
GEHE/ EuRho	Minoxidil	2109021-02	2
Gehe/Euro	Minoxidil	150903501	1
Gehe/EuRoh	Minoxidil	1907025-02	1
Gehe	Minoxidil		4
Gehe	Minoxidil	1405028-01	1
Gehe	Minoxidil	15436201	1
Gehe	Minoxidil	15436404	1
Gehe	Minoxidil	15436406	1
Gehe	Minoxidil	15436414	1
Gehe	Minoxidil	15K17-B06-321926	1
Gehe	Minoxidil	1602013-01	2
Gehe	Minoxidil	1612011-01	1
Gehe	Minoxidil	1705008-01	1
Gehe	Minoxidil	1710043-01	1
Gehe	Minoxidil	17227803	2
Gehe	Minoxidil	17H08-B06-341376	1
Gehe	Minoxidil	1803004-01	1
Gehe	Minoxidil	1807018-01	1
Gehe	Minoxidil	1901005-01	1
Gehe	Minoxidil	1907025-01	2
GEHE	Minoxidil	1907025-01	1
Gehe	Minoxidil	1907025-02	1
Gehe	Minoxidil	2004030-01	2
GEHE	Minoxidil	2109021-01	1
GEHE	Minoxidil	2209016-01	4
Gehe	Minoxidil	2209017-01	4
Gehe	Minoxidil	23H25-B13-234500	2
Gehe	Minoxidil	AP006/13M	1
Geibo	Minoxidil	1705008-01	1
Geilenkirchen	Minoxidil	14234505	1
Hedinger/Fiebig	Minoxidil	1612011-01	1
Hedinger/Noweda	Minoxidil	15436414	1
Hedinger/Sanacorp	Minoxidil	12C29-N05	1
Hedinger	Minoxidil	14B04-B07	2
Ichthyol/Noweda	Minoxidil	17117803	1
Ichthyol-Gesellschaft	Minoxidil	1311038-01	1
Icrom / Gehe	Minoxidil	20A15-B99-1966607	1
Icrom /Oberlinden-Ap...	Minoxidil	1/14	1
Icrom S.P.A./Sanacorp	Minoxidil	1907025-01	1
Icrom S.P.A./Sanacorp	Minoxidil	1907025-02	1
icrom spa	Minoxidil	511v	1
ICROM/Gehe	Minoxidil	12/17	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Icrom/Gehe	Minoxidil	1602013-01	1
ICROM	Minoxidil	6/12	1
Jenne	Minoxidil	17H08-B06-341377	2
Jenne	Minoxidil	B99-1966007	1
Jenne	Minoxidil	P2019/93	1
Kehr	Minoxidil	1705008-01	1
Kehr	Minoxidil	1803004-01	1
Krieger	Minoxidil	171004301	1
Krieger	Minoxidil	21B11-B20-210128	1
Kumar Cigan	Minoxidil	2004030-01	1
Kumar Organic Produc...	Minoxidil		1
Kumar Organics Products	Minoxidil	2001035-01	1
Kumar organics	Minoxidil	200804001	1
Kumar/Phoenix	Minoxidil		1
Laborchemie Apolda G...	Minoxidil	1803004-01	2
Moweda	Minoxidil	2311021-01	1
Noweda/ Infecto Pharm	Minoxidil	1607007-01	1
Noweda/Euro	Minoxidil	20080440-01	1
Noweda	Minoxidil	14093703	1
Noweda	Minoxidil	15K17-B05-320189	2
Noweda	Minoxidil	1705008-01	1
Noweda	Minoxidil	1710043-01	3
Noweda	Minoxidil	1803004-01	2
Noweda	Minoxidil	18149801	1
Noweda	Minoxidil	18149802	2
Noweda	Minoxidil	1901005-01	1
Noweda	Minoxidil	1907025-01	4
Noweda	Minoxidil	191957003	1
Noweda	Minoxidil	19E28-B12-193438	1
Noweda	Minoxidil	2004030-01	4
Noweda	Minoxidil	20040301	1
Noweda	Minoxidil	21002063012	1
Noweda	Minoxidil	210901801	1
Noweda	Minoxidil	2109018-01	1
Noweda	Minoxidil	2109021-02	1
Noweda	Minoxidil	22000546010	1
Oberlinden Apotheke	Minoxidil	5-13	1
Olon Spa	Minoxidil	15K17-B06-321926	1
Ph.Eur.10.0/Gehe	Minoxidil	2001035-01	1
phoenix /EuRho	Minoxidil	2004030-01	3
Phoenix	Minoxidil	1602013-02	1
Phoenix	Minoxidil	16J25-B05-332092	1
Phoenix	Minoxidil	2004030-01	1
Phoenix	Minoxidil	2008039-01	1
Phoenix	Minoxidil	2008040-01	1
Phoenix	Minoxidil	2109021-01	1
Phoenix	Minoxidil	21B02-B13-215374	1
Phoenix	Minoxidil	24B28-B11-236694	2
Phoenix	Minoxidil	3057	1
Phoenix	Minoxidil	3399	1
Phönix /euro	Minoxidil	170500801	2
Phönix/EuRho	Minoxidil	1710043-01	2
phönix	Minoxidil		1
Phönix	Minoxidil	1112024-03	1
Phönix	Minoxidil	1203035-02	1
Phönix	Minoxidil	1304029-01	1
Phönix	Minoxidil	1504013-01	1
phönix	Minoxidil	1509035-01	1
phönix	Minoxidil	1602013-01	3
Phönix	Minoxidil	1602013-02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
phönix	Minoxidil	1612011-01	2
Phönix	Minoxidil	1612011-01	1
Phönix	Minoxidil	170043-01	1
Phönix	Minoxidil	1705008-01	1
PHÖNIX	Minoxidil	1705008-01	2
Phönix	Minoxidil	18016109	1
Phönix	Minoxidil	18149815	1
Phönix	Minoxidil	1901005-01	1
Phönix	Minoxidil	1907025-01	2
Phönix	Minoxidil	19B21-B07-190661	1
Phönix	Minoxidil	2001030-01	1
Phönix	Minoxidil	2004030-01	5
PHÖNIX	Minoxidil	2004030-01	1
Phönix	Minoxidil	2008040-01	2
Phönix	Minoxidil	201062710	1
Phönix	Minoxidil	2109018-01	1
Phönix	Minoxidil	2209016-01	1
Phonix	Minoxidil	2311021-01	1
PHÖNIX	Minoxidil	CB2109018-01	1
Sana Eurho 11.11.19 ...	Minoxidil	1907025-01	1
sanacorb	Minoxidil	1612011-01	1
Sanacorp, 81,00EUR, 27.1.17	Minoxidil	1607007-01	1
Sanacorp/EuRho	Minoxidil	2001035-01	1
Sanacorp	Minoxidil	120056-01	1
Sanacorp	Minoxidil	1203035-01	1
Sanacorp	Minoxidil	1210056-01	1
Sanacorp	Minoxidil	1210056-02	2
Sanacorp	Minoxidil	1304029-02	3
Sanacorp	Minoxidil	13179501	2
Sanacorp	Minoxidil	13179502	2
Sanacorp	Minoxidil	13179507	1
sanacorp	Minoxidil	13K04-B05-290379	1
sanacorp	Minoxidil	1405028-01	1
Sanacorp	Minoxidil	140502801	1
Sanacorp	Minoxidil	1405028-01	1
Sanacorp	Minoxidil	14093701	1
Sanacorp	Minoxidil	14093702	1
Sanacorp	Minoxidil	1411006-01	1
Sanacorp	Minoxidil	1504013-01	1
Sanacorp	Minoxidil	1612011-01	1
Sanacorp	Minoxidil	180300401	1
Sanacorp	Minoxidil	1907025-01	1
Sanacorp	Minoxidil	191957010	1
Sanacorp	Minoxidil	2008040	1
Sanacorp	Minoxidil	2008040-01	2
Sanacorp	Minoxidil	20D27-B11-201218	1
Sanacorp	Minoxidil	21002063022	4
Sanacorp	Minoxidil	2109021-02	1
Sanacorp	Minoxidil	21b02-b13-215377	1
Sanacorp	Minoxidil	21B11-B18-203084	2
Sanacorp	Minoxidil	21F07-B05-215378	2
Sanacorp	Minoxidil	22000546001	1
Spangro 1.10.19	Minoxidil	16J24-B04-328224	1
Spangro 25.1.2014	Minoxidil	13/23-N07	1
Th. Geyer	Minoxidil	1602013-01	1
Vdl 14.07.14	Minoxidil	1311038-01	1
VDL;81,0EUR;21.05.15	Minoxidil	1411006-01	1

- 232 694 spectra from 1515 *Apo-Ident* customers from a total of 48 677 batches from a further

721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Minoxidil* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Minoxidil* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	579	0	152 383
Type B	0	1478	2	200 604
Type C	0	3362	11	232 694

The substance/substance group *Minoxidil* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9637 %)
Type B	100.0000 % (> 99.9912 %)	99.8649 % (> 99.6622 %)
Type C	100.0000 % (> 99.9007 %)	99.6739 % (> 99.5849 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20879	21630	7.45	195.66
21359	21630	5.53	195.22
21361	21630	5.06	195.77
21630	21630	0.00	195.41
21912	21933	5.08	196.67
21933	21933	0.00	193.02
22365	22365	0.00	198.76
22982	22982	0.00	200.92
25162	25162	0.00	197.43
25888	25888	0.00	198.96
26337	26337	0.00	200.20

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Mometasone furoate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20100-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mometasone furoate; Mometasoni furoas

Special notes

When selecting the *Mometasone furoate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Mometasone furoate	8	12	479

Second-stage model

For differentiation of the substance/substance group *Mometasone furoate* the following second-stage model is used:

- Submodel 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Mometasone furoate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Naloxone hydrochloride dihydrate	121.87	–
⋮	⋮	⋮
Atropine sulfate	>50	50.45
Potassium sorbate	>50	112.83
Magnesium hydrogen citrate	>50	130.56
Hydrocortisone	>50	173.97
Quinoline yellow	>50	262.50
Escin, water-soluble	>50	299.27
Propranolol hydrochloride	>50	310.00
Saccharin sodium	>50	405.28
Calcium orotate dihydrate	>50	524.82
Phenytoin	>50	529.64

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Mometasone furoate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Mometasone furoate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Mometasone furoate	160286	22433	60	20160316*
Caelo	Mometasone furoate	163532	23046	40	20170104*
Euro OTC	Mometasone furoate	1403015-01	21602	60	20140503
Euro OTC	Mometasone furoate	1403015-01	21602SI	31	20140503
Euro OTC	Mometasone furoate	1510036	22238	60	20151118*
Euro OTC	Mometasone furoate	1510036	22238SI	30	20151118*
Euro OTC	Mometasone furoate	1610009	23136	40	20170321*
Euro OTC	Mometasone furoate	2305005	26766	40	20230630*
Euro OTC	Mometasone furoate	2305005	26766SI	30	20230630*
Fagron	Mometasone furoate	13F17-N01	20850	40	20130620

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Mometasone furoate	13F17-N01	20850SI	44	20130620
Fagron	Mometasone furoate	16A20-B06-319750	22887	40	20160209
Fagron	Mometasone furoate	16A20-B06-319750	22887SI	30	20160209

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 545 spectra of 13 reference samples from the substance/substance group *Mometasone furoate*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 417 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 904 spectra of 27 reference samples from the substance/substance group *Mometasone furoate*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Mometasone furoate	13304605	21374	60
Caelo	Mometasone furoate	183341	24563	40
Caelo	Mometasone furoate	23001247	27248	40
Euro OTC	Mometasone furoate	1606021	22715	40
Euro OTC	Mometasone furoate	1711027	23878	40
Euro OTC	Mometasone furoate	1810008	24295	40
Euro OTC	Mometasone furoate	1906035	24794	40
Euro OTC	Mometasone furoate	2001040	25159	40
Euro OTC	Mometasone furoate	2003056	25167	40
Euro OTC	Mometasone furoate	2008002	25408	40
Euro OTC	Mometasone furoate	2106014	25869	50
Fagron	Mometasone furoate	22C15-B06-221102	26295	35

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Mometasone furoate	13304605	21374SI	38
Caelo	Mometasone furoate	160286	22433SI†	30
Caelo	Mometasone furoate	163532	23046SI†	23
Caelo	Mometasone furoate	183341	24563SI	21
Caelo	Mometasone furoate	23001247	27248SI	30
Euro OTC	Mometasone furoate	1606021	22715SI	33
Euro OTC	Mometasone furoate	1610009	23136SI†	20
Euro OTC	Mometasone furoate	1711027	23878SI	27
Euro OTC	Mometasone furoate	1810008	24295SI	20
Euro OTC	Mometasone furoate	1906035	24794SI	24
Euro OTC	Mometasone furoate	2001040	25159SI	30
Euro OTC	Mometasone furoate	2003056	25167SI	22
Euro OTC	Mometasone furoate	2008002	25408SI	20
Euro OTC	Mometasone furoate	2106014	25869SI	31
Fagron	Mometasone furoate	22C15-B06-221102	26295SI	30

- 201 180 spectra from a total of 4030 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2733 spectra from 769 *Apo-Ident* customers from 514 batches from the substance/substance group *Mometasone furoate*.
- Among them are spectra of independent samples from 478 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Mometasone furoate	20003486021	1
	Mometasone furoate	20003486024	4
	Mometasone furoate	20003486026	1
	Mometasone furoate	20003486027	1
	Mometasone furoate	20003486029	3
	Mometasone furoate	20003486030	4
	Mometasone furoate	20003486034	8
	Mometasone furoate	20003486035	8
	Mometasone furoate	20G24-B03-1968709	1
	Mometasone furoate	20G24-B03-197086	1
	Mometasone furoate	2106014-01	16
	Mometasone furoate	21B26-B05-203100	7
	Mometasone furoate	21B26-B05-2031000	1
	Mometasone furoate	22C15-B06-221102	1
	Mometasone furoate	22C15-B06-223109	1
	Mometasone furoate	22C15-B06-223110	1
	Mometasone furoate	22C15-B06-227594	3
	Mometasone furoate	23001247005	3
	Mometasone furoate	23001247006	3
	Mometasone furoate	2305005-01	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Mometasone furoate	24D10-B13-236853	1
	Mometasone furoate	B02-2346500	1
	Mometasone furoate	B03-1970806	2
AARTI / Gehe	Mometasone furoate	20000787001	1
AARTI Industries/Phoenix	Mometasone furoate	MF-18013(JM-01)-001	1
AARTI Industries/Phoenix	Mometasone furoate	MF-20002(JM-01)-001	1
Ador Pharma	Mometasone furoate	APMOM006/0517M	1
AEP	Mometasone furoate	20003486012	1
AHD 20.06.14 EK 37,29	Mometasone furoate	12C07-B05-291268	1
AHD/EuRho	Mometasone furoate	2001040-01	1
Alliance Health 27.0. . .	Mometasone furoate	13J23-N02	1
Alliance Healthcare	Mometasone furoate	B03-1968709	2
Alte Apotheke	Mometasone furoate	1606021-01	1
Anzag	Mometasone furoate	12J29N03	1
Anzag	Mometasone furoate	13D08-N06	1
Audor Pharma	Mometasone furoate	APMOM006/0117M	4
Audor Pharma	Mometasone furoate	APMOM006/0177M	1
Audor Pharma	Mometasone furoate	APMOM006/0517M	7
Audor Pharma	Mometasone furoate	APMOM010/0116M	3
Audor Pharma	Mometasone furoate	APMOM301/0118-1M	2
Audor Pharma	Mometasone furoate	APMOM301/0118-8M	1
Audor Pharma	Mometasone furoate	APMOM301/0118M	3
Beiersdorf	Mometasone furoate	18026011	1
Bombastus	Mometasone furoate	16J24-B11-335793	1
Bombastus	Mometasone furoate	18B19-B07-352632	1
Cael Sanacorp 05.02.2016	Mometasone furoate	14H06-B07-298481	1
Caelo	Mometasone furoate		1
Caelo	Mometasone furoate	116181714	1
Caelo	Mometasone furoate	12035601	1
Caelo	Mometasone furoate	12035607	2
Caelo	Mometasone furoate	12035608	2
Caelo	Mometasone furoate	12339604	1
Caelo	Mometasone furoate	12351202	1
Caelo	Mometasone furoate	12351205	2
Caelo	Mometasone furoate	12351207	1
Caelo	Mometasone furoate	12351208	1
Caelo	Mometasone furoate	12351210	1
Caelo	Mometasone furoate	12351215	4
Caelo	Mometasone furoate	13304603	1
Caelo	Mometasone furoate	13304604	2
Caelo	Mometasone furoate	13304605	4
Caelo	Mometasone furoate	13304606	4
Caelo	Mometasone furoate	13304609	1
Caelo	Mometasone furoate	13304612	1
Caelo	Mometasone furoate	13304614	1
Caelo	Mometasone furoate	13F27-N02	1
Caelo	Mometasone furoate	13H13N04	1
Caelo	Mometasone furoate	13H13-N04	1
Caelo	Mometasone furoate	13J23-N02	1
Caelo	Mometasone furoate	14281101	2
Caelo	Mometasone furoate	14281102	4
Caelo	Mometasone furoate	14281103	2
Caelo	Mometasone furoate	14C07-B05-291268	8
Caelo	Mometasone furoate	14E20-B04	1
Caelo	Mometasone furoate	14e20-b04-291267	1
Caelo	Mometasone furoate	14E20-B04-291267	1
Caelo	Mometasone furoate	14H06-B07298481	1
Caelo	Mometasone furoate	15/11-B02-314479	1
Caelo	Mometasone furoate	15/11-Bo2-314479	1
Caelo	Mometasone furoate	1510036-001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Mometasone furoate	151003601	1
Caelo	Mometasone furoate	1510036-02	2
Caelo	Mometasone furoate	15110301	4
Caelo	Mometasone furoate	15110305	4
Caelo	Mometasone furoate	15189801	3
Caelo	Mometasone furoate	15189802	5
Caelo	Mometasone furoate	15189804	3
Caelo	Mometasone furoate	15189806	1
Caelo	Mometasone furoate	15189807	5
Caelo	Mometasone furoate	15189809	5
Caelo	Mometasone furoate	15279003	1
Caelo	Mometasone furoate	15279004	6
Caelo	Mometasone furoate	15b11b03	1
Caelo	Mometasone furoate	15B11-B03-304121	2
Caelo	Mometasone furoate	15B11B03304122	1
Caelo	Mometasone furoate	15G08-B11-310864	2
Caelo	Mometasone furoate	15G08-B11-310865	1
Caelo	Mometasone furoate	15G08-B11-317182	1
Caelo	Mometasone furoate	15G08-B11-322739	1
Caelo	Mometasone furoate	1602809	1
Caelo	Mometasone furoate	16028601	4
Caelo	Mometasone furoate	16028602	7
Caelo	Mometasone furoate	16028604	6
Caelo	Mometasone furoate	16028605	2
Caelo	Mometasone furoate	16028606	7
Caelo	Mometasone furoate	16028607	8
Caelo	Mometasone furoate	16028609	9
Caelo	Mometasone furoate	1606021-01	6
Caelo	Mometasone furoate	1610009-01	8
Caelo	Mometasone furoate	16181703	1
Caelo	Mometasone furoate	16181704	8
Caelo	Mometasone furoate	16181705	4
Caelo	Mometasone furoate	16181708	4
Caelo	Mometasone furoate	16181709	6
Caelo	Mometasone furoate	16181710	5
Caelo	Mometasone furoate	16181714	1
Caelo	Mometasone furoate	16181715	7
Caelo	Mometasone furoate	1635206	1
Caelo	Mometasone furoate	1635209	1
Caelo	Mometasone furoate	1635211	1
Caelo	Mometasone furoate	16353201	7
Caelo	Mometasone furoate	16353204	2
Caelo	Mometasone furoate	16353205	4
Caelo	Mometasone furoate	16353206	14
Caelo	Mometasone furoate	16353207	15
Caelo	Mometasone furoate	16353208	5
Caelo	Mometasone furoate	16353209	20
Caelo	Mometasone furoate	16353210	4
Caelo	Mometasone furoate	16353211	14
Caelo	Mometasone furoate	16353212	2
Caelo	Mometasone furoate	1653205	1
Caelo	Mometasone furoate	16A20-B06-319748	1
Caelo	Mometasone furoate	16A20-B06-319749	1
Caelo	Mometasone furoate	16C24_B03_324852	2
Caelo	Mometasone furoate	16C24-B03-324852	1
Caelo	Mometasone furoate	16C24-B03-327346	1
Caelo	Mometasone furoate	16C24-B03-328272	1
Caelo	Mometasone furoate	16J24-B11	1
Caelo	Mometasone furoate	16J24-B11-332112	1
Caelo	Mometasone furoate	16J24B11-334371	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Mometasone furoate	16J24-B11-334371	2
Caelo	Mometasone furoate	16J24-B11-335793	1
Caelo	Mometasone furoate	1704012A	1
Caelo	Mometasone furoate	1711027	1
Caelo	Mometasone furoate	1711027-01	1
Caelo	Mometasone furoate	17348901	10
Caelo	Mometasone furoate	17D19-B02	3
Caelo	Mometasone furoate	17D19-B02-339277	1
Caelo	Mometasone furoate	17D19-B02-342643	3
Caelo	Mometasone furoate	17D19-B02-34476	1
Caelo	Mometasone furoate	17D19-B02-347348	2
Caelo	Mometasone furoate	17D1-B02-344776	1
Caelo	Mometasone furoate	18026001	24
Caelo	Mometasone furoate	18026002	1
Caelo	Mometasone furoate	18026003	5
Caelo	Mometasone furoate	18026004	16
Caelo	Mometasone furoate	18026005	1
Caelo	Mometasone furoate	18026006	6
Caelo	Mometasone furoate	18026007	9
Caelo	Mometasone furoate	18026008	5
Caelo	Mometasone furoate	18026009	3
Caelo	Mometasone furoate	18026010	1
Caelo	Mometasone furoate	18026011	23
Caelo	Mometasone furoate	18026012	14
Caelo	Mometasone furoate	18026015	6
Caelo	Mometasone furoate	18026017	6
Caelo	Mometasone furoate	1802603	1
Caelo	Mometasone furoate	1802611	1
Caelo	Mometasone furoate	1806012	1
Caelo	Mometasone furoate	1810008-01	2
Caelo	Mometasone furoate	18102013B	1
Caelo	Mometasone furoate	18334101	9
Caelo	Mometasone furoate	18334102	19
Caelo	Mometasone furoate	18334103	1
Caelo	Mometasone furoate	18334104	20
Caelo	Mometasone furoate	18334106	12
Caelo	Mometasone furoate	18334108	9
Caelo	Mometasone furoate	18334109P-191111-4	1
Caelo	Mometasone furoate	18334110	13
Caelo	Mometasone furoate	18B19B07-351001	1
Caelo	Mometasone furoate	18B19-B07-351351	1
Caelo	Mometasone furoate	18B19-B07-352632	1
Caelo	Mometasone furoate	18B19-B07-354319	1
Caelo	Mometasone furoate	18B-B07-354320	1
Caelo	Mometasone furoate	192006004	7
Caelo	Mometasone furoate	19200601	21
Caelo	Mometasone furoate	19200602	19
Caelo	Mometasone furoate	19200603	14
Caelo	Mometasone furoate	19200604	5
Caelo	Mometasone furoate	19200605	9
Caelo	Mometasone furoate	19F13-B12-191761	1
Caelo	Mometasone furoate	200000787008	1
Caelo	Mometasone furoate	200003486010	1
Caelo	Mometasone furoate	2000078004	1
Caelo	Mometasone furoate	20000787001	21
Caelo	Mometasone furoate	20000787002	1
Caelo	Mometasone furoate	20000787004	17
Caelo	Mometasone furoate	20000787005	20
Caelo	Mometasone furoate	20000787007	12
Caelo	Mometasone furoate	20000787008	8

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Mometasone furoate	20000787009	1
Caelo	Mometasone furoate	20000787010	9
Caelo	Mometasone furoate	20000787012	15
Caelo	Mometasone furoate	20000787013	8
Caelo	Mometasone furoate	2000078787001	1
Caelo	Mometasone furoate	2000346006	1
Caelo	Mometasone furoate	20003486002	12
Caelo	Mometasone furoate	20003486004	34
Caelo	Mometasone furoate	20003486005	1
Caelo	Mometasone furoate	20003486006	15
Caelo	Mometasone furoate	20003486009	3
Caelo	Mometasone furoate	20003486010	11
Caelo	Mometasone furoate	20003486011	15
Caelo	Mometasone furoate	20003486012	10
Caelo	Mometasone furoate	20003486013	1
Caelo	Mometasone furoate	20003486016	10
Caelo	Mometasone furoate	20003486017	7
Caelo	Mometasone furoate	20003486018	10
Caelo	Mometasone furoate	20003486021	6
Caelo	Mometasone furoate	20003486024	13
Caelo	Mometasone furoate	20003486026	3
Caelo	Mometasone furoate	20003486027	4
Caelo	Mometasone furoate	20003486030	3
Caelo	Mometasone furoate	20003486035	1
Caelo	Mometasone furoate	20003486036	1
Caelo	Mometasone furoate	200034866016	1
Caelo	Mometasone furoate	200034896004	1
Caelo	Mometasone furoate	2000787001	1
Caelo	Mometasone furoate	2000787004	1
Caelo	Mometasone furoate	2000787007	1
Caelo	Mometasone furoate	2000787013	1
Caelo	Mometasone furoate	200315A	1
Caelo	Mometasone furoate	2003486026	1
Caelo	Mometasone furoate	20g24-b03-196879	1
Caelo	Mometasone furoate	20G24-B03-196879	1
Caelo	Mometasone furoate	220003486026	1
Caelo	Mometasone furoate	240913a	1
Caelo	Mometasone furoate	2885	1
Caelo	Mometasone furoate	34860062	1
Caelo	Mometasone furoate	701834-0002	1
Caelo	Mometasone furoate	9530001	1
Caelo	Mometasone furoate	9530018	1
Caelo	Mometasone furoate	APMOM006/0117M	1
Caelo	Mometasone furoate	MOM001/0317	1
Caelo	Mometasone furoate	MOM010/0116	3
Caelo	Mometasone furoate	NO1352M	1
Caelo	Mometasone furoate	NT1568M	1
Caelo	Mometasone furoate	NU0698M	1
Caelo	Mometasone furoate	NV1000M	1
Caeo/Noweda	Mometasone furoate	15279003	1
Caeo	Mometasone furoate	12351201	1
Caeolo/Gehe	Mometasone furoate	16J24-B11-332112	1
Caeolo/Gehe	Mometasone furoate	18334104	1
Caesa / Alliance Hea...	Mometasone furoate	18026012	1
Caesar & Lorenz GmbH	Mometasone furoate	18334108	1
Caesar & Lorenz GmbH	Mometasone furoate	20000787001	1
Caesar & Loretz GmbH...	Mometasone furoate	2000078005	1
Caesar & Loretz GmbH...	Mometasone furoate	18026015	1
Caesar & Loretz GmbH...	Mometasone furoate	20000787005	1
Caesar & Loretz GmbH...	Mometasone furoate	11H10-N04	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/ AHD	Mometasone furoate	20003486016	1
Caesar & Loretz GmbH...	Mometasone furoate	20000787005	1
Caesar & Loretz GmbH...	Mometasone furoate	20003486017	2
Caesar & Loretz GmbH...	Mometasone furoate	20003486010	1
Caesar & Loretz GmbH/AHD	Mometasone furoate	20003486006	1
Caesar & Loretz GmbH...	Mometasone furoate	20003486006	2
Caesar & Loretz GmbH...	Mometasone furoate	20003486021	1
Caesar & Loretz GmbH/Gehe	Mometasone furoate	19200605	1
Caesar & Loretz GmbH/Gehe	Mometasone furoate	20003486016	1
Caesar & Loretz GmbH...	Mometasone furoate	20003486004	4
Caesar & Loretz GmbH...	Mometasone furoate	18334108	1
Caesar & Loretz GmbH...	Mometasone furoate	20000787001	1
Caesar & Loretz GmbH...	Mometasone furoate	20003486026	1
Caesar & Loretz GmbH...	Mometasone furoate	20003486034	1
Caesar & Loretz GmbH...	Mometasone furoate	20000787001	1
Caesar & Loretz GmbH...	Mometasone furoate	20003486024	1
Caesar & Loretz GmbH/Otto	Mometasone furoate	20000787010	1
Caesar & Loretz GmbH/Ph	Mometasone furoate	20003486018	1
Caesar & Loretz GmbH...	Mometasone furoate	2000078712	1
Caesar & Loretz GmbH...	Mometasone furoate	20003486002	1
Caesar & Loretz GmbH...	Mometasone furoate	20003486004	1
Caesar & Loretz GmbH...	Mometasone furoate	20000787008	1
Caesar & Loretz GmbH...	Mometasone furoate	20003486011	1
Caesar & Loretz GmbH/S	Mometasone furoate	20003486010	1
Caesar & Loretz GmbH/S	Mometasone furoate	20003486024	1
Caesar & Loretz GmbH/Sa	Mometasone furoate	18334108	1
Caesar & Loretz GmbH/Sa	Mometasone furoate	19200601	1
Caesar & Loretz GmbH/Sana	Mometasone furoate	20003486012	1
Caesar & Loretz GmbH...	Mometasone furoate	20003486010	1
Caesar & Loretz GmbH...	Mometasone furoate	20003486018	2
Caesar & Loretz GmbH...	Mometasone furoate	20003486024	1
Caesar & Loretz GmbH	Mometasone furoate	12035601	1
Caesar & Loretz GmbH	Mometasone furoate	16028609	2
Caesar & Loretz GmbH	Mometasone furoate	18026001	1
Caesar & Loretz GmbH	Mometasone furoate	18026012	5
Caesar & Loretz GmbH	Mometasone furoate	18026013	1
Caesar & Loretz GmbH	Mometasone furoate	18026014	1
Caesar & Loretz GmbH	Mometasone furoate	18026017	1
Caesar & Loretz GmbH	Mometasone furoate	18072120	1
Caesar & Loretz GmbH	Mometasone furoate	18334101	4
Caesar & Loretz GmbH	Mometasone furoate	18334102	3
Caesar & Loretz GmbH	Mometasone furoate	18334104	4
Caesar & Loretz GmbH	Mometasone furoate	18334106	2
Caesar & Loretz GmbH	Mometasone furoate	18334108	8
Caesar & Loretz GmbH	Mometasone furoate	18334110	3
Caesar & Loretz GmbH	Mometasone furoate	19200601	4
Caesar & Loretz GmbH	Mometasone furoate	19200602	2
Caesar & Loretz GmbH	Mometasone furoate	19200603	2
Caesar & Loretz GmbH	Mometasone furoate	19200604	1
Caesar & Loretz GmbH	Mometasone furoate	19200605	7
Caesar & Loretz GmbH	Mometasone furoate	200003486024	1
Caesar & Loretz GmbH	Mometasone furoate	20000787001	8
Caesar & Loretz GmbH	Mometasone furoate	20000787002	1
Caesar & Loretz GmbH	Mometasone furoate	20000787004	2
Caesar & Loretz GmbH	Mometasone furoate	20000787005	4
Caesar & Loretz GmbH	Mometasone furoate	20000787007	3
Caesar & Loretz GmbH	Mometasone furoate	20000787008	2
Caesar & Loretz GmbH	Mometasone furoate	20000787010	4
Caesar & Loretz GmbH	Mometasone furoate	20000787012	2
Caesar & Loretz GmbH	Mometasone furoate	20000787013	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Mometasone furoate	20003486002	11
Caesar & Loretz GmbH	Mometasone furoate	20003486004	14
Caesar & Loretz GmbH	Mometasone furoate	20003486006	8
Caesar & Loretz GmbH	Mometasone furoate	20003486008	4
Caesar & Loretz GmbH	Mometasone furoate	20003486010	1
Caesar & Loretz GmbH	Mometasone furoate	20003486011	11
Caesar & Loretz GmbH	Mometasone furoate	20003486012	3
Caesar & Loretz GmbH	Mometasone furoate	20003486016	3
Caesar & Loretz GmbH	Mometasone furoate	20003486017	5
Caesar & Loretz GmbH	Mometasone furoate	20003486018	8
Caesar & Loretz GmbH	Mometasone furoate	20003486020	1
Caesar & Loretz GmbH	Mometasone furoate	20003486021	12
Caesar & Loretz GmbH	Mometasone furoate	20003486024	2
Caesar & Loretz GmbH	Mometasone furoate	20003486026	2
Caesar & Loretz GmbH	Mometasone furoate	20003486027	2
Caesar & Loretz GmbH	Mometasone furoate	2001040-01	2
Caesar & Loretz GmbH	Mometasone furoate	22C15-B06-221102	1
Caesar & Loretz GmbH	Mometasone furoate	30000787007	1
Caesar & Loretz GmbH	Mometasone furoate	B03-1968709	1
Caesar & Loretz GmbH	Mometasone furoate	B03-1970806	1
Caesar & Loretz Hilden	Mometasone furoate	18026012	1
Caesar & Loretz/Geil…	Mometasone furoate	20003486006	2
Caesar & Loretz/Noweda	Mometasone furoate	18026012	1
Caesar u Loretz	Mometasone furoate	15279004	2
Caesar u. Loretz GmbH	Mometasone furoate	19200605	1
Caesar und Loretz GmbH	Mometasone furoate	2000787010	1
caesar&Loretz GmbH,P…	Mometasone furoate	16028604	1
Caesar&loretz,AHC,08…	Mometasone furoate		1
Calo/AHD	Mometasone furoate	19200603	1
Carlo/Phönix/21,89	Mometasone furoate	18334102	1
Cealo/Anzag	Mometasone furoate	18026012	1
Cealo	Mometasone furoate	20003486004	2
EuRho / 2	Mometasone furoate	1906035-01	1
EuRho / 2	Mometasone furoate	2003056-01	1
EuRho / Noweda	Mometasone furoate	1906035-01	2
EuRho/AHD	Mometasone furoate	2003056-01	1
EuRho/AHD	Mometasone furoate	2008002-01	3
EuRho/Gehe	Mometasone furoate	2001040-01	1
EuRho/Gehe	Mometasone furoate	2106014-01	1
EuRho/Ph	Mometasone furoate	2001040-01	2
EuRho/Phönix	Mometasone furoate	1307037-01	2
EuRho	Mometasone furoate	1408010-01	1
EuRho	Mometasone furoate	15/11-B02-315705	1
Eurho	Mometasone furoate	18B19-B07-352744	1
EuRho	Mometasone furoate	2003056-01	1
EuRho	Mometasone furoate	2008002-01	1
Euro OTC	Mometasone furoate		2
Euro OTC	Mometasone furoate	1203024-02	1
Euro OTC	Mometasone furoate	1307037-01	1
Euro OTC	Mometasone furoate	1408010-01	2
Euro OTC	Mometasone furoate	1504012-01	7
Euro OTC	Mometasone furoate	1504012-02	5
Euro OTC	Mometasone furoate	1510036-01	15
Euro OTC	Mometasone furoate	15G08-B11-317182	1
Euro OTC	Mometasone furoate	15G08-B11-322738	2
Euro OTC	Mometasone furoate	160009-01	1
Euro OTC	Mometasone furoate	160602101	1
Euro OTC	Mometasone furoate	1606021-01	8
Euro OTC	Mometasone furoate	16100009-01	3
Euro OTC	Mometasone furoate	1610009-001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Mometasone furoate	161000901	1
Euro OTC	Mometasone furoate	1610009-01	27
Euro OTC	Mometasone furoate	16J24-b11	1
Euro OTC	Mometasone furoate	16j24-B11-332111	1
Euro OTC	Mometasone furoate	1711027	1
Euro OTC	Mometasone furoate	171102701	1
Euro OTC	Mometasone furoate	1711027-01	9
Euro OTC	Mometasone furoate	1711027-02	4
Euro OTC	Mometasone furoate	17D19-B02-342643	1
Euro OTC	Mometasone furoate	17D19B02347349	1
Euro OTC	Mometasone furoate	18026006	1
Euro OTC	Mometasone furoate	1810002-01	1
Euro OTC	Mometasone furoate	1810008_01	1
Euro OTC	Mometasone furoate	181000801	2
Euro OTC	Mometasone furoate	1810008-01	28
Euro OTC	Mometasone furoate	1810008-01P-200331-2	1
Euro OTC	Mometasone furoate	18334108	1
Euro OTC	Mometasone furoate	18B19-B07-352632	1
Euro OTC	Mometasone furoate	19060035	1
Euro OTC	Mometasone furoate	1906035	2
Euro OTC	Mometasone furoate	190603501	2
Euro OTC	Mometasone furoate	1906035-01	31
Euro OTC	Mometasone furoate	20008002-01	1
Euro OTC	Mometasone furoate	2001040-01	15
Euro OTC	Mometasone furoate	2003056-01	45
Euro OTC	Mometasone furoate	200800-01	1
Euro OTC	Mometasone furoate	200800201	4
Euro OTC	Mometasone furoate	2008002-01	86
Euro OTC	Mometasone furoate	2106014-01	30
Euro OTC	Mometasone furoate	23051822	1
Euro OTC	Mometasone furoate	5991	1
Euro OTC	Mometasone furoate	83919-23-7	1
Euro OTG	Mometasone furoate	1403015-01	1
EURO/Noweda	Mometasone furoate	2003056-01	1
EuRoh/ Gehe	Mometasone furoate	2008002-01	1
Fagr/sana EK: EUR 39,2...	Mometasone furoate	18B19-B07-35151	1
Fagro/Noweda	Mometasone furoate	17D19-B02-339277	1
Fagro	Mometasone furoate	1511B02	1
Fagron	Mometasone furoate		1
Fagron	Mometasone furoate	10805-N12	1
Fagron	Mometasone furoate	10C29-N10	1
Fagron	Mometasone furoate	10E31-N26	1
Fagron	Mometasone furoate	11C02-N03	2
Fagron	Mometasone furoate	11F08-N03	1
Fagron	Mometasone furoate	11H10-N01	1
Fagron	Mometasone furoate	11h10-n04	1
Fagron	Mometasone furoate	11H10-N04	2
Fagron	Mometasone furoate	11K28-N09	2
Fagron	Mometasone furoate	12B22-N01	1
Fagron	Mometasone furoate	12B22-N04	1
Fagron	Mometasone furoate	12e02-n11	1
Fagron	Mometasone furoate	12E02-N11	4
Fagron	Mometasone furoate	12H09-N02	7
Fagron	Mometasone furoate	12I29-N03	1
Fagron	Mometasone furoate	12J29-N01	1
Fagron	Mometasone furoate	12J29-N03	4
Fagron	Mometasone furoate	13d08-n06	1
Fagron	Mometasone furoate	13D08N06	1
Fagron	Mometasone furoate	13D08-N06	14
Fagron	Mometasone furoate	13Do8-N06	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Mometasone furoate	13f17-n01	1
Fagron	Mometasone furoate	13F17-N01	9
Fagron	Mometasone furoate	13F27-N02	7
Fagron	Mometasone furoate	13F27-NO2	1
Fagron	Mometasone furoate	13F7-N01	1
Fagron	Mometasone furoate	13H13-N04	10
Fagron	Mometasone furoate	13H13-NO4	1
Fagron	Mometasone furoate	13j23_n02	1
Fagron	Mometasone furoate	13j23-N02	1
Fagron	Mometasone furoate	13J23-N02	21
Fagron	Mometasone furoate	13j23-no2	1
Fagron	Mometasone furoate	140305MF	1
Fagron	Mometasone furoate	14C07-B05-291264	1
Fagron	Mometasone furoate	14C07-B05-291266	2
Fagron	Mometasone furoate	14C07-B05-291268	5
Fagron	Mometasone furoate	14E20-B04	4
Fagron	Mometasone furoate	14e20b04291265	1
Fagron	Mometasone furoate	14e20-b04-291265	1
Fagron	Mometasone furoate	14E20-B04-291265	3
Fagron	Mometasone furoate	14e20-b04-291267	1
Fagron	Mometasone furoate	14E20-B04-291267	7
Fagron	Mometasone furoate	14E20-B04-291269	2
Fagron	Mometasone furoate	14E20-B04-291271	1
Fagron	Mometasone furoate	14E20-B04-294645	7
Fagron	Mometasone furoate	14E20-B04-302374	2
Fagron	Mometasone furoate	14H06-B07297240	1
Fagron	Mometasone furoate	14H06-B07-297240	3
Fagron	Mometasone furoate	14H06-B07-298481	2
Fagron	Mometasone furoate	14H06-B07-298482	7
Fagron	Mometasone furoate	14H06-B07-302375	2
Fagron	Mometasone furoate	14H06-B07-302376	3
Fagron	Mometasone furoate	15/11-B02	4
Fagron	Mometasone furoate	15/11-B02-314479	5
Fagron	Mometasone furoate	15/11B02315705	2
Fagron	Mometasone furoate	15/11-B02-315705	3
Fagron	Mometasone furoate	15/11-B02-316705	1
Fagron	Mometasone furoate	15B11-B03	2
Fagron	Mometasone furoate	15b11-b03-304120	1
Fagron	Mometasone furoate	15B11-B03-304120	7
Fagron	Mometasone furoate	15B11B03304121	1
Fagron	Mometasone furoate	15B11-B03-304121	9
Fagron	Mometasone furoate	15B11B03304122	1
Fagron	Mometasone furoate	15B11-B03-304122	6
Fagron	Mometasone furoate	15B11-B03-304123	14
Fagron	Mometasone furoate	15b11-b03-304124	1
Fagron	Mometasone furoate	15B11-B03-304124	2
Fagron	Mometasone furoate	15b11-b03-308276	2
Fagron	Mometasone furoate	15B11-B03-308276	3
Fagron	Mometasone furoate	15B11B03308860	1
Fagron	Mometasone furoate	15B11-B03-308860	2
Fagron	Mometasone furoate	15G08	1
Fagron	Mometasone furoate	15G08-B11	3
Fagron	Mometasone furoate	15G08-B11-0002	1
Fagron	Mometasone furoate	15G08-B11-310864	8
Fagron	Mometasone furoate	15G08-B11-312233	4
Fagron	Mometasone furoate	15G08-B11-317182	9
Fagron	Mometasone furoate	15G08-B11-322737	2
Fagron	Mometasone furoate	15g08-b11-322738	1
Fagron	Mometasone furoate	15G08B11322738	1
Fagron	Mometasone furoate	15G08-B11-322738	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Mometasone furoate	15G-B11-310864	1
Fagron	Mometasone furoate	15I11-B02-314479	4
Fagron	Mometasone furoate	15I11-B02-315705	1
Fagron	Mometasone furoate	15J11-B02-315705	1
Fagron	Mometasone furoate	16/24-B11-332122	1
Fagron	Mometasone furoate	16181709	1
Fagron	Mometasone furoate	16181714	1
Fagron	Mometasone furoate	16724-B11-332112	1
Fagron	Mometasone furoate	16A20-B06	3
Fagron	Mometasone furoate	16A20-B06-319740	1
Fagron	Mometasone furoate	16A20-B06-319748	7
Fagron	Mometasone furoate	16A20-B06319749	1
Fagron	Mometasone furoate	16A20-B06-319749	6
Fagron	Mometasone furoate	16A20-B06-322739	6
Fagron	Mometasone furoate	16A20-Bo6-319748	1
Fagron	Mometasone furoate	16C24	1
Fagron	Mometasone furoate	16C24-803-324851	1
Fagron	Mometasone furoate	16C24B03	1
Fagron	Mometasone furoate	16C24-B03	3
Fagron	Mometasone furoate	16C24B03324851	1
Fagron	Mometasone furoate	16C24-B03-324851	4
Fagron	Mometasone furoate	16C24B03324852	1
Fagron	Mometasone furoate	16C24-B03-324852	5
Fagron	Mometasone furoate	16C24-B03-325575	1
Fagron	Mometasone furoate	16C24-B03-326790	10
Fagron	Mometasone furoate	16C24-B03-327346	4
Fagron	Mometasone furoate	16c24-b03-327372	1
Fagron	Mometasone furoate	16C24-b03-327372	1
Fagron	Mometasone furoate	16C24-B03-327372	5
Fagron	Mometasone furoate	16C24-B03-328272	6
Fagron	Mometasone furoate	16J24-11-335793	1
Fagron	Mometasone furoate	16j24-b11	1
Fagron	Mometasone furoate	16J24-B11	6
Fagron	Mometasone furoate	16j24-b11-329817	1
Fagron	Mometasone furoate	16J24B11329817	1
Fagron	Mometasone furoate	16J24-B11-329817	4
Fagron	Mometasone furoate	16J24-B11-330978	5
Fagron	Mometasone furoate	16J24-B11-332110	3
Fagron	Mometasone furoate	16J24-B11-332111	5
Fagron	Mometasone furoate	16J24B11332112	1
Fagron	Mometasone furoate	16J24-B11-332112	14
Fagron	Mometasone furoate	16J24B11334371	1
Fagron	Mometasone furoate	16J24-B11-334371	9
Fagron	Mometasone furoate	16j24-b11-335792	1
Fagron	Mometasone furoate	16J24-B11-335792	1
Fagron	Mometasone furoate	16j24b11335793	1
Fagron	Mometasone furoate	16J24B11335793	1
Fagron	Mometasone furoate	16J24-B11-335793	11
Fagron	Mometasone furoate	17D1834	1
Fagron	Mometasone furoate	17D19	1
Fagron	Mometasone furoate	17D19_B02_339278	1
Fagron	Mometasone furoate	17D19-B02	5
Fagron	Mometasone furoate	17D19-B02_339278	1
Fagron	Mometasone furoate	17D19-B02-33927	2
Fagron	Mometasone furoate	17D19-B02-339276	3
Fagron	Mometasone furoate	17D19B02339277	1
Fagron	Mometasone furoate	17D19-B02339277	1
Fagron	Mometasone furoate	17D19-B02-339277	4
Fagron	Mometasone furoate	17D19-B02-339278	6
Fagron	Mometasone furoate	17D19B02342642	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Mometasone furoate	17D19-B02-342642	3
Fagron	Mometasone furoate	17D19-B02-342643	20
Fagron	Mometasone furoate	17D19-B02-344776	3
Fagron	Mometasone furoate	17D19-B02-347347	5
Fagron	Mometasone furoate	17D19-B02-347348	5
Fagron	Mometasone furoate	17d19-b02-347349	1
Fagron	Mometasone furoate	17D19B02347349	1
Fagron	Mometasone furoate	17D19-B02-347349	15
Fagron	Mometasone furoate	17D19-B02-3477347	1
Fagron	Mometasone furoate	1814E3640	1
Fagron	Mometasone furoate	18819-807	1
Fagron	Mometasone furoate	18819-b07	1
Fagron	Mometasone furoate	18819-B07-345319	1
Fagron	Mometasone furoate	18819-B07-356278	1
Fagron	Mometasone furoate	18819-B07-357640	3
Fagron	Mometasone furoate	18B199-B07-354320	1
Fagron	Mometasone furoate	18B19-B07	10
Fagron	Mometasone furoate	18B19-B07-341351	1
Fagron	Mometasone furoate	18b19-b07-351001	1
Fagron	Mometasone furoate	18B19-B07-351001	1
Fagron	Mometasone furoate	18B19-B07-351351	9
Fagron	Mometasone furoate	18b19-b07-352632	1
Fagron	Mometasone furoate	18B19B07352632	1
Fagron	Mometasone furoate	18B19-B07-352632	17
Fagron	Mometasone furoate	18B19-B07-352635	1
Fagron	Mometasone furoate	18B19-B07-352744	9
Fagron	Mometasone furoate	18B19B07352745	1
Fagron	Mometasone furoate	18B19-B07-352745	13
Fagron	Mometasone furoate	18B19-B07-354318	4
Fagron	Mometasone furoate	18B19-B07-354319	5
Fagron	Mometasone furoate	18B19-B07-354319MOM010/0118	1
Fagron	Mometasone furoate	18B19-B07-354320	19
Fagron	Mometasone furoate	18B19-B07-357228	3
Fagron	Mometasone furoate	18B19-B07-357640	11
Fagron	Mometasone furoate	191761	2
Fagron	Mometasone furoate	19200604	1
Fagron	Mometasone furoate	197086	1
Fagron	Mometasone furoate	19F13B12191760	2
Fagron	Mometasone furoate	19F13-B12-191760	5
Fagron	Mometasone furoate	19F13B12191761	1
Fagron	Mometasone furoate	19F13-B12-191761	22
Fagron	Mometasone furoate	19F13-B12-1917610481	1
Fagron	Mometasone furoate	19F13-B12-191762	8
Fagron	Mometasone furoate	19F13-B191761	1
Fagron	Mometasone furoate	20000787001	1
Fagron	Mometasone furoate	20G24_B03-197086	1
Fagron	Mometasone furoate	20G244-B03-196879	1
Fagron	Mometasone furoate	20g24-803-196879	1
Fagron	Mometasone furoate	20G24-B03	11
Fagron	Mometasone furoate	20G24-B03-1968709	1
Fagron	Mometasone furoate	20G24-B03-196879	27
Fagron	Mometasone furoate	20G24B03197086	4
Fagron	Mometasone furoate	20G24-B03-197086	23
Fagron	Mometasone furoate	20G24-B03-201311	2
Fagron	Mometasone furoate	20G24-B03-196879	2
Fagron	Mometasone furoate	20G24-B03-201311	1
Fagron	Mometasone furoate	210543	1
Fagron	Mometasone furoate	2114M3640	1
Fagron	Mometasone furoate	21B26-B05	2
Fagron	Mometasone furoate	21b26-b05-203100	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Mometasone furoate	21B26-B05-203100	22
Fagron	Mometasone furoate	21B26-B05-203101	14
Fagron	Mometasone furoate	21B26B05210542	1
Fagron	Mometasone furoate	21B26-B05-210542	6
Fagron	Mometasone furoate	21B26-B05-210543	7
Fagron	Mometasone furoate	21B26-B05-213869	1
Fagron	Mometasone furoate	21B26-B05-219115	1
Fagron	Mometasone furoate	21B26-B05-219200	1
Fagron	Mometasone furoate	21B26-BO5-213869	1
Fagron	Mometasone furoate	2215I-07030	1
Fagron	Mometasone furoate	22C15-B06-219423	2
Fagron	Mometasone furoate	22C15B06221102	1
Fagron	Mometasone furoate	22C15-B06-221102	3
Fagron	Mometasone furoate	22C15-B06-223110	3
Fagron	Mometasone furoate	22C15-B06-227594	1
Fagron	Mometasone furoate	22C15-BO6-221102	1
Fagron	Mometasone furoate	2517Q-07030	1
Fagron	Mometasone furoate	2714U-07030	1
Fagron	Mometasone furoate	2818A-07030	1
Fagron	Mometasone furoate	3313A-07030	1
Fagron	Mometasone furoate	334371	1
Fagron	Mometasone furoate	335793	1
Fagron	Mometasone furoate	339278	1
Fagron	Mometasone furoate	347349	2
Fagron	Mometasone furoate	352632	1
Fagron	Mometasone furoate	354319	1
Fagron	Mometasone furoate	4(18B19-B07-351001	1
Fagron	Mometasone furoate	5(MOM001/0220)	1
Fagron	Mometasone furoate	5/0715	1
Fagron	Mometasone furoate	6071716	1
Fagron	Mometasone furoate	701834-0001	1
Fagron	Mometasone furoate	701834-0004	1
Fagron	Mometasone furoate	83919-23-7	3
Fagron	Mometasone furoate	B03-1968709	7
Fagron	Mometasone furoate	B03-1970806	5
Fagron	Mometasone furoate	B03-197086	2
Fagron	Mometasone furoate	B05-2031001	2
Fagron	Mometasone furoate	B05-2105403	1
Fagron	Mometasone furoate	B12-1917600	1
Fagron	Mometasone furoate	BO3-1968709	1
Fagron	Mometasone furoate	Fagron21B26-B05-203101	1
Fagron	Mometasone furoate	HM01620	1
Fagron	Mometasone furoate	HMF010620	1
Fagron	Mometasone furoate	HMF01620	2
Fagron	Mometasone furoate	HMFO1620	1
Fagron	Mometasone furoate	mom001/0220	1
Fagron	Mometasone furoate	MOM001/0220	9
Fagron	Mometasone furoate	MOM001/0317	4
Fagron	Mometasone furoate	MOM003/0818	6
Fagron	Mometasone furoate	MOM004/0716	4
Fagron	Mometasone furoate	MOM004-0716	1
Fagron	Mometasone furoate	MOM008/0915	3
Fagron	Mometasone furoate	MOM010/0116	2
Fagron	Mometasone furoate	MOM010/0118	8
Fagron	Mometasone furoate	NS1513M	1
Fagron	Mometasone furoate	NT1568M	3
Fagron	Mometasone furoate	NU0698M	2
Fagron	Mometasone furoate	NU2504M	1
Fargo / Gehe	Mometasone furoate	20G24-B03	1
Fargon/AHD	Mometasone furoate	18B19-B07-351001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fargon/AHD	Mometasone furoate	18B19-B07-354319	1
Fargon/Gehe	Mometasone furoate	20G24-B03-197086	2
Fargon	Mometasone furoate	13H13-N04	1
Fargon	Mometasone furoate	14h06-b07-298481	2
Fargon	Mometasone furoate	16C24-B03-324852	1
Fargon	Mometasone furoate	20G24-B03-196879	1
Fargron/Noweda	Mometasone furoate	20G24-B03-197086	1
Finteler Apotheke	Mometasone furoate	16028603	1
Finteler Apotheke	Mometasone furoate	16028604	1
Fragon/Phoenix	Mometasone furoate	19F13-B12-191762	1
Fragon/Sanacorp	Mometasone furoate	16C24-B03-324851	1
Fragon/Sanacorp	Mometasone furoate	17D19-B02-339277	2
Fragon/Sanacorp	Mometasone furoate	17D19-B02-342642	1
Fragon/Sanacorp	Mometasone furoate	17D19-B02-342643	2
Fragon/Sanacorp	Mometasone furoate	17D19-B02-347348	1
Fragron/ Alliance	Mometasone furoate	20G24-B03-196879	1
Gehe 07.12.18	Mometasone furoate	1711027_02	1
GEHE 17.04.2014	Mometasone furoate	13J23-N02	1
Gehe amax	Mometasone furoate	17D19-B02-342643	1
Gehe amax	Mometasone furoate	1906035-01	1
Gehe amax	Mometasone furoate	19F13-B12-191761	1
Gehe/Caesar & Loretz GmbH	Mometasone furoate	20003486021	1
Gehe/EuRoh	Mometasone furoate	2003056-01	1
Gehe/europharm	Mometasone furoate	2106014-01	6
Gehe	Mometasone furoate	13D08-N06	1
Gehe	Mometasone furoate	13H13-N04	2
Gehe	Mometasone furoate	15B11-B03-304123	1
Gehe	Mometasone furoate	15G08-B11-312233	1
Gehe	Mometasone furoate	15G08-B11-317182	1
Gehe	Mometasone furoate	16181704	1
Gehe	Mometasone furoate	16353201	1
Gehe	Mometasone furoate	16353206	1
Gehe	Mometasone furoate	16353207	1
Gehe	Mometasone furoate	16C24-B03-324852	1
Gehe	Mometasone furoate	16C24-B03-327346	1
Gehe	Mometasone furoate	16J24-B11-332112	2
Gehe	Mometasone furoate	16J24-B11-335793	2
Gehe	Mometasone furoate	17D19-B02	1
Gehe	Mometasone furoate	17D19-B02-339278	1
Gehe	Mometasone furoate	17D19-B02-342642	2
GEHE	Mometasone furoate	17D19-B02-344776	1
GEHE	Mometasone furoate	18026006	1
Gehe	Mometasone furoate	18334101	1
gehe	Mometasone furoate	18334104	1
Gehe	Mometasone furoate	18B19-B07-352745	4
Gehe	Mometasone furoate	18B19-B07-354318	1
Gehe	Mometasone furoate	18B19-B07-354319	1
Gehe	Mometasone furoate	18B19-B07-354319	1
Gehe	Mometasone furoate	1906035-01	3
Gehe	Mometasone furoate	19F13-B12-191761	1
Gehe	Mometasone furoate	20003486002	1
Gehe	Mometasone furoate	20003486026	1
Gehe	Mometasone furoate	20003486034	1
gehe	Mometasone furoate	20G24-Bo3-196879	1
Gehe	Mometasone furoate	22C15-B06-221102	1
Geibo/ Fargron	Mometasone furoate	16J24-b11-335792	1
Geibo	Mometasone furoate	18B19-B07-354320	1
GUMO	Mometasone furoate	2008002-01	5
Hedinger/Gehe	Mometasone furoate	1896223	1
Holdermann	Mometasone furoate	13D08-N06	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Holdermann	Mometasone furoate	14C07-B05-29126	1
Ichthyol-Gesllschaft...	Mometasone furoate	16J24-B11-335793	2
Jenne	Mometasone furoate	18026012	1
Jenne	Mometasone furoate	1802612	1
Jenne	Mometasone furoate	20003486030	1
Jenne	Mometasone furoate	20003486034	1
Jenne	Mometasone furoate	21B26-805-203100	1
Kehr	Mometasone furoate	16353206	1
Nachprüfung	Mometasone furoate	1628604	1
Nachprüfung	Mometasone furoate	16J24-B11-329817	1
Newchem / Gehe	Mometasone furoate	16181715	1
Noveda	Mometasone furoate	18334101	1
Noveda	Mometasone furoate	20000787010	1
Noweda /Cealo	Mometasone furoate	19200601	2
Noweda Taucha	Mometasone furoate	20003486011	1
Noweda Taucha	Mometasone furoate	2008002-01	2
Noweda	Mometasone furoate	15G08-B11	1
Noweda	Mometasone furoate	16C24-B03-328272	1
Noweda	Mometasone furoate	16J24-B11-332111	1
Noweda	Mometasone furoate	1711027-02	1
Noweda	Mometasone furoate	17D19-B02-347349	1
Noweda	Mometasone furoate	18026009	1
Noweda	Mometasone furoate	18334110	1
Noweda	Mometasone furoate	18B19-B07-351351	1
Noweda	Mometasone furoate	20G24-B03-196879	1
Noweda	Mometasone furoate	2106014-01	4
Noweda	Mometasone furoate	21B26-B05-203100	2
Noweda	Mometasone furoate	22C-B06	1
Noweda	Mometasone furoate	23001247006	1
Phagron	Mometasone furoate	19F13-B12-191761	1
Phoenix 03.08.2017	Mometasone furoate	16C24-B03-328272	1
Phoenix	Mometasone furoate	14C07-B05-291268	1
Phoenix	Mometasone furoate	16181714	1
Phoenix	Mometasone furoate	17D19-B02-339277	1
Phoenix	Mometasone furoate	1810008-01	1
phoenix	Mometasone furoate	18334108	1
Phoenix	Mometasone furoate	18B19-B07-352745	1
Phoenix	Mometasone furoate	19F13-B12-191760	1
Phoenix	Mometasone furoate	20003486036	1
phoenix	Mometasone furoate	2008002-01	1
Phoenix	Mometasone furoate	20G24-B03-196879	1
Phoenix	Mometasone furoate	3406	1
Phoenix	Mometasone furoate	MOM004/0716	1
Phönix Gotha	Mometasone furoate	1403015-01	1
Phönix	Mometasone furoate	13/23-N02	2
Phönix	Mometasone furoate	13D08-N06	1
Phönix	Mometasone furoate	14E20-B04-291267	1
phönix	Mometasone furoate	15B11-b03	1
Phönix	Mometasone furoate	15G08-B11-322737	1
Phönix	Mometasone furoate	16C24-B03	1
Phönix	Mometasone furoate	16c24-b03-327346	1
Phönix	Mometasone furoate	171102702	1
Phönix	Mometasone furoate	17D19-B02-342642	1
Phönix	Mometasone furoate	18026012	1
Phönix	Mometasone furoate	1906035-01	2
Phönix	Mometasone furoate	20003486017	1
Phönix	Mometasone furoate	20003486018	1
Phönix	Mometasone furoate	2008002-01	4
Phönix	Mometasone furoate	20G24-B03	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
phönix	Mometasone furoate	2106014-01	1
Phönix	Mometasone furoate	2106014-01	1
Phönx	Mometasone furoate	2008002-01	3
Sana	Mometasone furoate	MF-18009(JM-01)001	1
Sanacorp /Fargron	Mometasone furoate	15G08-B11-310864	1
Sanacorp /Fargron	Mometasone furoate	16J24-B11-335792	1
Sanacorp	Mometasone furoate	1/AKD4	1
Sanacorp	Mometasone furoate	14E20-B04-291267	1
Sanacorp	Mometasone furoate	15189801	1
Sanacorp	Mometasone furoate	16353211	1
Sanacorp	Mometasone furoate	17D19-B02-339276	1
Sanacorp	Mometasone furoate	17D19-B02-344776	2
Sanacorp	Mometasone furoate	18026001	1
Sanacorp	Mometasone furoate	18B19-B07-354319	2
Sanacorp	Mometasone furoate	20000787007	1
Sanacorp	Mometasone furoate	20G24-B03-197086	2
Sanacorp	Mometasone furoate	21B26-B05	1
Sanacorp	Mometasone furoate	21B26-B05-203100	2
Sanacorp	Mometasone furoate	22C15-B06-227594	1
Sanacorp	Mometasone furoate	23001247006	1
Sanacorp	Mometasone furoate	23F15-B02-234650	1
Sanacorp	Mometasone furoate	MOM001/0317	1
SanacorpWE:12.01.201…	Mometasone furoate	16028602	1
sidonia	Mometasone furoate	18334110	1
Symbiotic/Phoenix	Mometasone furoate	2001040-01	2
Symbiotica / Gehe	Mometasone furoate	MOM008/0915	2
Symbiotica Malaysia/ AHD	Mometasone furoate	2001040-01	1
Symbiotica/Phoenix	Mometasone furoate	MOM001/0317	1
Symbiotica/Phoenix	Mometasone furoate	MOM003/0818	2

- 233 334 spectra from 1514 *Apo-Ident* customers from a total of 48 750 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Mometasone furoate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mometasone furoate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	545	0	152 417
Type B	0	903	1	201 180
Type C	0	2724	9	233 334

The substance/substance group *Mometasone furoate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8991 %)
Type B	100.0000 % (> 99.9912 %)	99.8894 % (> 99.5575 %)
Type C	100.0000 % (> 99.9007 %)	99.6707 % (> 99.5609 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20850	22433	5.72	180.74
21602	22433	9.36	181.96
22238	22238	0.00	179.21
22433	22433	0.00	183.20
22887	23136	8.35	182.86
23046	23046	0.00	178.85
23136	23136	0.00	182.43
26766	26766	0.00	183.34

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Monostereates**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20691-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Monostereates; Glycerol monostearate 40-55; Glycerol monostearate 60; Glycerol monostearate, emulsifying; Glyceroli monostearas 40–55; Glyceroli monostearates 60; Glyceroli monostearates emulsificantes; Sorbitan stearate; Sorbitani stearas

Special notes

When selecting the *Monostereates* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Monostereates	37	19	141

Second-stage model

For differentiation of the substance/substance group *Monostereates* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Monostereates* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Emulsifying cetostearyl alcohol (type A)	48.60	–
Non-ionic emulsifying alcohol	52.15	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Monostereates* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Monostereates*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Glycerol monostearate 40-55	12105705	20691	80	20120424
Caelo	Glycerol monostearate 40-55	12105720	20867	40	20120424
Caelo	Glycerol monostearate 40-55	14099903	21446	60	AR-15-FG-000732-02
Caelo	Glycerol monostearate 40-55	154450	22464	60	20160225*
Caelo	Glycerol monostearate 40-55	20002884	25620	40	20200916*
Caelo	Glycerol monostearate 40-55	22000532	26018	40	20220331*
Caelo	Glycerol monostearate 40-55	23000431	26729	40	20230526*
Caelo	Glycerol monostearate 40-55	23000431	26729SI	20	20230526*
Fagron	Glycerol monostearate 40-55	14C12-B40-292622	21545	60	20140404
Fagron	Glycerol monostearate 40-55	15E13-B03-305532	22277	60	20150703
Caelo	Glycerol monostearate 60	13109304	21093	40	1407633
Caelo	Glycerol monostearate 60	13232604	21437	60	1504599
Caelo	Glycerol monostearate 60	15286302	21982	60	20150911
Caelo	Glycerol monostearate 60	15286302	22320	60	AR-16-FG-009226-01
Caelo	Glycerol monostearate 60	16233804	23188	40	10052
Caelo	Glycerol monostearate 60	180683	24025	40	20180430*
Caelo	Glycerol monostearate 60	182462	24371	40	20181008*
Caelo	Glycerol monostearate 60	190547	24673	40	20190423*
Caelo	Glycerol monostearate 60	192857002	25385	40	20191216
Caelo	Glycerol monostearate 60	21003001	26004	40	20211109*
Caelo	Glycerol monostearate 60	21003001	26004SI	30	20211109*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Glycerol monostearate 60	22003434	26728	40	20230213*
Caelo	Glycerol monostearate 60	22003434	26728SI	20	20230213*
Caelo	Glycerol monostearate 60	24001839	27316	40	20240829*
Caelo	Glycerol monostearate 60	24001839	27316SI	20	20240829*
Caelo	Glycerol monostearate, em…	12210401	20751	80	1407214
Caelo	Glycerol monostearate, em…	12210401	20783	40	20120726
Caelo	Glycerol monostearate, em…	14240607	21576	60	1412120
Caelo	Glycerol monostearate, em…	14240607	21585	60	20140815
Caelo	Glycerol monostearate, em…	161646	22623	40	20160727*
Caelo	Glycerol monostearate, em…	16030301	22667	40	20160204
Caelo	Glycerol monostearate, em…	21000650	25618	40	20210310*
Caelo	Glycerol monostearate, em…	21002557002	26235	40	20210920
Caelo	Glycerol monostearate, em…	21002557002	26235SI	20	20210920
Caelo	Glycerol monostearate, em…	22003075	26480	40	20221121*
Caelo	Glycerol monostearate, em…	22003075	26480SI	20	20221121*
Caelo	Glycerol monostearate, em…	23002137	26958	40	20230829*
Caelo	Glycerol monostearate, em…	23002137	26958SI	20	20230829*
Caelo	Sorbitan stearate	12274801	20828	40	20120924
Caelo	Sorbitan stearate	162352	22764	40	20160826*
Caelo	Sorbitan stearate	17030805	23706	40	20170210
Caelo	Sorbitan stearate	172564	23831	40	20171027*
Caelo	Sorbitan stearate	192928	25094	40	20191122*
Caelo	Sorbitan stearate	20002274	25564	40	20201009*
Caelo	Sorbitan stearate	22002437	26369	40	20220819*
Caelo	Sorbitan stearate	22002437	26369SI	20	20220819*
Caelo	Sorbitan stearate	24000967	27257	40	20240529*
Fagron	Sorbitan stearate	14J07-B02-299399	21885	60	AR-16-FG-004368-01

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 2050 spectra of 48 reference samples from the substance/substance group *Monostereates*. These samples are listed above in the *calibration samples* section. The reference samples come from 37 different batches.
- 150 912 spectra from a total of 2805 batches from further 480 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1210 spectra of 29 reference samples from the substance/substance group *Monostereates*.
- Among them are spectra of independent samples from 19 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Glycerol monostearate 40-55	180447	24267	40
Caelo	Glycerol monostearate 40-55	190794	24709	40
Caelo	Glycerol monostearate 40-55	191186	24713	40
Caelo	Glycerol monostearate 40-55	24000632	27255	40
Caelo	Glycerol monostearate 60	11272902	20677	80
Caelo	Glycerol monostearate 60	162338	22646	40
Caelo	Glycerol monostearate 60	20002478	25505	40
Caelo	Glycerol monostearate, em…	14308310	21993	60
Caelo	Glycerol monostearate, em…	172585	23822	40
Fagron	Glycerol monostearate, em…	11I15-N09	20746	80
Fagron	Glycerol monostearate, em…	12B14-N10	20786	40
Caelo	Sorbitan stearate	171781	23622	40
Caelo	Sorbitan stearate	180432	24021	40
Caelo	Sorbitan stearate	183125	24377	40
Caelo	Sorbitan stearate	192168	24900	40
Caelo	Sorbitan stearate	21001797	25807	50
Caelo	Sorbitan stearate	21004159	25991	40
Caelo	Sorbitan stearate	24002443	27435	40
Fagron	Sorbitan stearate	11I26-N09	20736	40
Caelo	Glycerol monostearate 40-55	22000532	26018SI†	10
Caelo	Glycerol monostearate 40-55	24000632	27255SI	20
Caelo	Glycerol monostearate 60	162338	22741	40
Caelo	Glycerol monostearate 60	162338	22742	40
Caelo	Glycerol monostearate 60	162338	22743	40
Caelo	Glycerol monostearate 60	162338	22744	40
Caelo	Glycerol monostearate, em…	14308310	22278	60
Caelo	Glycerol monostearate, em…	14308310	22341	60
Caelo	Sorbitan stearate	21004159	25991SI	10
Caelo	Sorbitan stearate	24000967	27257SI†	20

- 200 874 spectra from a total of 4024 batches from further 835 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 447 spectra from 226 *Apo-Ident* customers from 148 batches from the substance/substance group *Monostereates*.
- Among them are spectra of independent samples from 136 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Supplier	Substance	Batch	Spectra
	Glycerol monostearate 40-55	22000532003	1
	Glycerol monostearate 60	22001891001	1
	Glycerol monostearate 60	22001891004	1
	Sorbitan stearate	22002437005	1
	Sorbitan stearate	22002437008	1
	Sorbitan stearate	22003955002	1
	Sorbitan stearate	23000412001	1
	Glycerol monostearate 60	23001269003	1
ALH	Sorbitan stearate	16235202	1
Alliance	Sorbitan stearate	21004159001	1
Anzag	Glycerol monostearate 60	12180502	1
anzag	Sorbitan stearate	14195	1
Audor Pharma	Glycerol monostearate 60	13232604	1
Bombastus	Glycerol monostearate 40-55	18044701	1
Caelo	Glycerol monostearate 60		1
Caelo	Glycerol monostearate, em...	11079308	1
Caelo	Glycerol monostearate 60	12001001	1
Caelo	Glycerol monostearate 40-55	12105704	1
Caelo	Glycerol monostearate 40-55	12105729	1
Caelo	Glycerol monostearate 60	12180502	1
Caelo	Sorbitan stearate	12274807	1
Caelo	Sorbitan stearate	12274813	2
Caelo	Glycerol monostearate 60	13018201	3
Caelo	Glycerol monostearate 60	1301821	1
Caelo	Glycerol monostearate 60	13109304	9
Caelo	Glycerol monostearate, em...	13109402	1
Caelo	Glycerol monostearate, em...	13109405	2
Caelo	Glycerol monostearate, em...	13109410	1
Caelo	Glycerol monostearate 40-55	131156602	1
Caelo	Glycerol monostearate 40-55	13156601	2
Caelo	Sorbitan stearate	13209409	2
Caelo	Sorbitan stearate	13209410	1
Caelo	Sorbitan stearate	13209417	3
Caelo	Sorbitan stearate	13209418	2
Caelo	Sorbitan stearate	13209419	3
Caelo	Glycerol monostearate 40-55	13221303	2
Caelo	Glycerol monostearate 40-55	13221308	1
Caelo	Glycerol monostearate 60	13232604	3
Caelo	Sorbitan stearate	13B19-N01	1
Caelo	Glycerol monostearate 60	14012002	4
Caelo	Sorbitan stearate	14038504	1
Caelo	Sorbitan stearate	14038510	1
Caelo	Sorbitan stearate	14038511	2
Caelo	Glycerol monostearate 40-55	14169710	1
Caelo	Glycerol monostearate, em...	1420607	1
Caelo	Sorbitan stearate	14218803	3
Caelo	Sorbitan stearate	14218804	1
Caelo	Sorbitan stearate	14218808	5
Caelo	Sorbitan stearate	14218809	1
Caelo	Glycerol monostearate, em...	14240607	1
Caelo	Glycerol monostearate, em...	14240611	1
Caelo	Glycerol monostearate, em...	14308310	4
Caelo	Glycerol monostearate 40-55	14359407	2
Caelo	Sorbitan stearate	14372803	1
Caelo	Glycerol monostearate 60	15009203	13
Caelo	Glycerol monostearate 40-55	15130501	1
Caelo	Glycerol monostearate 40-55	15280902	1
Caelo	Glycerol monostearate 40-55	15280903	2
Caelo	Glycerol monostearate 40-55	15280904	2
Caelo	Glycerol monostearate 40-55	15280912	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glycerol monostearate 60	15286302	4
Caelo	Glycerol monostearate 60	15286307	2
Caelo	Glycerol monostearate 60	15286308	4
Caelo	Sorbitan stearate	15300302	7
Caelo	Sorbitan stearate	15300308	5
Caelo	Sorbitan stearate	15415202	9
Caelo	Glycerol monostearate 40-55	15445007	6
Caelo	Glycerol monostearate 40-55	15445010	1
Caelo	Glycerol monostearate 40-55	15445011	1
Caelo	Glycerol monostearate 40-55	15445014	2
Caelo	Glycerol monostearate, em…	16030301	3
Caelo	Glycerol monostearate, em…	16030304	2
Caelo	Glycerol monostearate, em…	16164604	1
Caelo	Glycerol monostearate, em…	16164606	1
Caelo	Glycerol monostearate 60	16233802	2
Caelo	Glycerol monostearate 60	16233804	6
Caelo	Sorbitan stearate	16235202	5
Caelo	Sorbitan stearate	16235207	11
Caelo	Sorbitan stearate	17030805	7
Caelo	Sorbitan stearate	17030806	2
Caelo	Glycerol monostearate 60	17061703	5
Caelo	Glycerol monostearate 60	17167803	7
Caelo	Glycerol monostearate 60	17167804	6
Caelo	Sorbitan stearate	17178102	21
Caelo	Glycerol monostearate, em…	17258501	2
Caelo	Glycerol monostearate, em…	17258505	2
Caelo	Sorbitan stearate	17345402	6
Caelo	Sorbitan stearate	17345403P-181005-2	1
Caelo	Sorbitan stearate	17345403P-181227-8	1
Caelo	Glycerol monostearate 40-55	18044701	2
Caelo	Glycerol monostearate 40-55	18044702	1
Caelo	Glycerol monostearate 60	18068303	3
Caelo	Sorbitan stearate	18204705	8
Caelo	Glycerol monostearate 60	18246203	3
Caelo	Glycerol monostearate 60	18246207	5
Caelo	Sorbitan stearate	18312504P-190502-1	1
Caelo	Sorbitan stearate	18312504P-190627-8	1
Caelo	Sorbitan stearate	18312507P-191230-1	1
Caelo	Glycerol monostearate, em…	18328702	4
Caelo	Glycerol monostearate, em…	18328705	2
Caelo	Glycerol monostearate 40-55	18334601	1
Caelo	Glycerol monostearate 40-55	18334601P-190405-2	1
Caelo	Glycerol monostearate 60	19054702	13
Caelo	Glycerol monostearate 40-55	190794001	2
Caelo	Glycerol monostearate 40-55	19079401	8
Caelo	Sorbitan stearate	19101301	1
Caelo	Sorbitan stearate	19101302P-190718-8	1
Caelo	Sorbitan stearate	19101302P-190926-7	1
Caelo	Sorbitan stearate	19101305	4
Caelo	Sorbitan stearate	19101306P-200326-8	1
Caelo	Sorbitan stearate	19101306P-200709-5	1
Caelo	Glycerol monostearate 60	191258003	7
Caelo	Glycerol monostearate, em…	192039002	6
Caelo	Glycerol monostearate, em…	192039003	1
Caelo	Sorbitan stearate	192168003	1
Caelo	Glycerol monostearate 60	192857001	1
Caelo	Glycerol monostearate 60	192857002	2
Caelo	Sorbitan stearate	20001211004	1
Caelo	Glycerol monostearate 40-55	20001564002	2
Caelo	Glycerol monostearate 60	20002478004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Glycerol monostearate 40-55	200028840001	1
Caelo	Glycerol monostearate 40-55	20002884001	1
Caelo	Glycerol monostearate 40-55	20002884002	1
Caelo	Sorbitan stearate	20003871004	1
Caelo	Glycerol monostearate 60	21000650001	6
Caelo	Glycerol monostearate, em...	21000650004	1
Caelo	Glycerol monostearate, em...	2100065001	1
Caelo	Glycerol monostearate 60	21001621002	5
Caelo	Glycerol monostearate 60	21001621004	3
Caelo	Sorbitan stearate	21001797001	3
Caelo	Glycerol monostearate, em...	21002557002	1
Caelo	Glycerol monostearate 60	21003001004	7
Caelo	Sorbitan stearate	21004159001	1
Caelo	Sorbitan stearate	22001545003	1
Caelo	Sorbitan stearate	26031507	1
Caelo	Glycerol monostearate 60	7035059	1
Caesar & Loretz GmbH...	Glycerol monostearate, em...	21000650001	1
Caesar & Loretz GmbH...	Sorbitan stearate	22001545003	1
Caesar & Loretz GmbH/Gehe	Sorbitan stearate	20003871007	1
Caesar & Loretz GmbH/Kehr	Sorbitan stearate	20003871004	1
Caesar & Loretz GmbH...	Glycerol monostearate 60	19054702	1
Caesar & Loretz GmbH...	Sorbitan stearate	18204705	1
Caesar & Loretz GmbH...	Glycerol monostearate 60	18246203	1
Caesar & Loretz GmbH/Sa	Glycerol monostearate 40-55	19079404	1
Caesar & Loretz GmbH/Sa	Glycerol monostearate 40-55	20001564002	1
Caesar & Loretz GmbH...	Sorbitan stearate	19101301	1
Caesar & Loretz GmbH...	Sorbitan stearate	21001797001	1
Caesar & Loretz GmbH	Glycerol monostearate 60	18068303	1
Caesar & Loretz GmbH	Sorbitan stearate	18204705	1
Caesar & Loretz GmbH	Glycerol monostearate, em...	18328702	1
Caesar & Loretz GmbH	Glycerol monostearate 40-55	18328705	1
Caesar & Loretz GmbH	Glycerol monostearate 60	19054702	3
Caesar & Loretz GmbH	Glycerol monostearate 40-55	19079401	2
Caesar & Loretz GmbH	Sorbitan stearate	19101305	1
Caesar & Loretz GmbH	Glycerol monostearate 60	191258003	2
Caesar & Loretz GmbH	Glycerol monostearate 40-55	192039002	1
Caesar & Loretz GmbH	Sorbitan stearate	192168003	2
Caesar & Loretz GmbH	Glycerol monostearate 60	192857002	3
Caesar & Loretz GmbH	Sorbitan stearate	20001211004	1
Caesar & Loretz GmbH	Glycerol monostearate 40-55	20003935003	1
Caesar & Loretz GmbH	Glycerol monostearate 60	21001621002	1
Caesar & Loretz GmbH	Glycerol monostearate 60	21001621004	1
Caesar & Loretz GmbH	Glycerol monostearate, em...	21002557002	4
Caesar & Loretz GmbH	Glycerol monostearate 40-55	22000532003	1
Caesar & Loretz GmbH	Glycerol monostearate 40-55	22000532004	1
Caesar & Loretz GmbH	Sorbitan stearate	22001545003	1
Caesar & Loretz GmbH	Sorbitan stearate	22002437005	1
Caesar & Loretz Hild...	Sorbitan stearate	19101305	1
Caesar & Loretz/Noweda	Glycerol monostearate 60	15009203	1
Caesar u Loretz	Glycerol monostearate 60	13109304	1
Caesar u Loretz	Glycerol monostearate 60	14012002	1
Caesar&Loretz GmbH/Gehe	Glycerol monostearate, em...	17258505	1
Caesar/Noweda	Glycerol monostearate 60	13109304	1
Caesar/Noweda	Glycerol monostearate 40-55	13221311	2
cealo sanacorp	Glycerol monostearate 60	20002478004	1
Cealo	Sorbitan stearate	13209409	1
Euro OTC	Glycerol monostearate 60	16233804	1
Fagron	Glycerol monostearate 40-55	12A27-N11	1
Fagron	Sorbitan stearate	12E30-N14	1
Fagron	Glycerol monostearate 40-55	12K05-N06	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Sorbitan stearate	13B19-N01	1
Fagron	Sorbitan stearate	13D10_N10	1
Fagron	Sorbitan stearate	13D10-N10	1
Fagron	Sorbitan stearate	14J07-B02-299399	1
Fagron	Glycerol monostearate 60	15009203	1
Fagron	Glycerol monostearate 40-55	15280903	1
Fagron	Sorbitan stearate	5052	1
Fagron	Glycerol monostearate 40-55	7G19-N09	1
Fiebig	Glycerol monostearate 40-55	20001564002	1
Gehe	Glycerol monostearate, em…	14240605	2
Gehe	Glycerol monostearate, em…	18328702	1
Gehe	Glycerol monostearate 60	19054702	1
Gehe	Glycerol monostearate 40-55	20001564002	1
Ichthyol/Phoenix	Sorbitan stearate	14372803	1
Krieger	Glycerol monostearate 60	19054702	1
L12	Glycerol monostearate 60	16233802	2
Nachprüfung	Sorbitan stearate		1
Noweda	Glycerol monostearate, em…	11079301	1
Noweda	Glycerol monostearate 60	15009203	1
Noweda	Sorbitan stearate	17178102	1
Noweda	Sorbitan stearate	21001797001	1
Noweda	Sorbitan stearate	22002437005	1
Phonix	Glycerol monostearate 60	13109304	1
Phonix	Sorbitan stearate	13209418	1
Sanacorp	Sorbitan stearate	22002437005	1
Spangropharm	Glycerol monostearate 40-55	80402468	1

- 235 620 spectra from 1515 *Apo-Ident* customers from a total of 49 112 batches from a further 718 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Monostereates* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Monostereates* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	2050	0	150 912
Type B	0	1209	1	200 874
Type C	0	446	1	235 620

The substance/substance group *Monostereates* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.7073 %)
Type B	100.0000 % (> 99.9912 %)	99.9174 % (> 99.6694 %)
Type C	100.0000 % (> 99.9007 %)	99.7763 % (> 99.1051 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20691	21446	21.72	66.52
20751	20751	0.00	153.56
20783	20751	4.30	149.31
20828	22764	35.32	96.29
20867	21446	33.82	71.16
21093	21093	0.00	108.44
21437	21437	0.00	100.42
21446	21446	0.00	65.58
21545	21446	31.93	70.40
21576	21576	0.00	133.58
21585	21576	2.50	134.30
21885	21885	0.00	116.72
21982	22320	6.24	104.61
22277	25620	23.13	61.38
22320	22320	0.00	103.67
22464	22464	0.00	73.06
22623	22623	0.00	128.58
22667	20751	18.95	169.11
22764	22764	0.00	96.43
23188	23188	0.00	91.19
23706	22764	6.44	98.37
23831	23831	0.00	111.23
24025	24025	0.00	122.34
24371	24371	0.00	120.74
24673	24673	0.00	123.56
25094	25094	0.00	101.21
25385	22320	30.72	125.33
25564	25564	0.00	102.87
25618	25618	0.00	120.96
25620	25620	0.00	61.12
26004	26004	0.00	107.12
26018	26018	0.00	73.42
26235	25618	20.73	127.88
26369	26369	0.00	111.01
26480	26480	0.00	122.53
26728	26728	0.00	101.67
26729	26729	0.00	61.87
26958	26958	0.00	123.84

continued on the next page

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
27257	27257	0.00	112.29
27316	27316	0.00	114.43

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Mupirocin calcium**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20781-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Mupirocin calcium; Mupirocinum calcicum

Special notes

When selecting the *Mupirocin calcium* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Mupirocin calcium	8	4	14

Second-stage model

For differentiation of the substance/substance group *Mupirocin calcium* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Mupirocin calcium* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	85.18	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Mupirocin calcium* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Mupirocin calcium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Mupirocin calcium	14276602	21745	60	20141103
Caelo	Mupirocin calcium	161184	22454	60	20160504*
Caelo	Mupirocin calcium	18191606	25376	40	20180813
Caelo	Mupirocin calcium	23003561	27116	40	20240202*
Caelo	Mupirocin calcium	23003561	27116SI	20	20240202*
Fagron	Mupirocin calcium	12E02-N07	20781	40	1401556
Fagron	Mupirocin calcium	15H13-B01-316111	23213	40	20150909
Fagron	Mupirocin calcium	18A16-B02-349169	25373	40	20180226
Fagron	Mupirocin calcium	21K17-B01-219626	26152	40	20220426
Fagron	Mupirocin calcium	21K17-B01-219626	26152SI	20	20220426

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 400 spectra of 10 reference samples from the substance/substance group *Mupirocin calcium*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 562 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 5 reference samples from the substance/substance group *Mupirocin calcium*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Mupirocin calcium	161608	23860	40
Caelo	Mupirocin calcium	21003209003	25856	50
Caelo	Mupirocin calcium	22001500	26259	40
Euro OTC	Mupirocin calcium	2001029	25297	40
Caelo	Mupirocin calcium	22001500	26259SI	20

- 201 894 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 14 spectra from 11 *Apo-Ident* customers from 14 batches from the substance/substance group *Mupirocin calcium*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Mupirocin calcium	17356502	1
Caelo	Mupirocin calcium	17356506	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Mupirocin calcium	17356509	1
Caelo	Mupirocin calcium	17F21-B03-34519	1
Caelo	Mupirocin calcium	18191601	1
Caelo	Mupirocin calcium	24041801	1
Caelo	Mupirocin calcium	83200301013	1
Caelo	Mupirocin calcium	9041801	1
Fagron	Mupirocin calcium	14B03-B30-297291	1
Fagron	Mupirocin calcium	15H13-B01	1
Fagron	Mupirocin calcium	17F21-B03	1
Fagron	Mupirocin calcium	17F21-B03-338597	1
Fagron	Mupirocin calcium	17F21-B03-339080	1
Fagron	Mupirocin calcium	83200340116	1

- 236 053 spectra from 1515 *Apo-Ident* customers from a total of 49 244 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Mupirocin calcium* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Mupirocin calcium* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	190	0	201 894
Type C	0	14	0	236 053

The substance/substance group *Mupirocin calcium* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20781	20781	0.00	102.63
21745	22454	14.30	102.69
22454	22454	0.00	103.62
23213	27116	13.65	104.69
25373	27116	36.88	105.83
25376	27116	9.75	104.19
26152	27116	16.93	105.45
27116	27116	0.00	104.38

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**myo-Inositol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20420-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

myo-Inositol; myo-Inositolum

Special notes

When selecting the *myo-Inositol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
myo-Inositol	3	1	6

Second-stage model

For differentiation of the substance/substance group *myo-Inositol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *myo-Inositol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	76.22	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *myo-Inositol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *myo-Inositol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	myo-Inositol	1206032-01	21280	40	20120814
Fagron	myo-Inositol	13D15-B40-328250	23405	40	20140812
Fagron	myo-Inositol	13D15-B40-328250	23406	40	AR-17-FG-016393-01
Fagron	myo-Inositol	23D12-B07-223058	26730	40	20230517
Fagron	myo-Inositol	23D12-B07-223058	26730SI	20	20230517

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 5 reference samples from the substance/substance group *myo-Inositol*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 152 782 spectra from a total of 2839 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *myo-Inositol*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	myo-Inositol	18A03-B04-344527	23999	40

- 202 044 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 6 *Apo-Ident* customers from 6 batches from the substance/substance group *myo-Inositol*.
- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	myo-Inositol	L1609025-01	1
Euro OTC	myo-Inositol	130400901	1
Euro OTC	myo-Inositol	1304009-01	1
Euro OTC	myo-Inositol	1609025-01	1
Euro OTC	myo-Inositol	L2010021-01	1
Fagron	myo-Inositol	L13090200	1

- 236 061 spectra from 1515 *Apo-Ident* customers from a total of 49 252 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *myo-Inositol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *myo-Inositol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	180	0	152 782
Type B	0	40	0	202 044
Type C	0	6	0	236 061

The substance/substance group *myo-Inositol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21280	23406	5.70	185.03
23405	23406	3.07	176.22
23406	23406	0.00	176.57
26730	23406	6.59	184.86

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Naloxone hydrochloride dihydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20957-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Naloxone hydrochloride dihydrate; Naloxoni hydrochloridum dihydricum

Special notes

When selecting the *Naloxone hydrochloride dihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Naloxone hydrochloride dihydrate	9	8	43

Second-stage model

For differentiation of the substance/substance group *Naloxone hydrochloride dihydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Naloxone hydrochloride dihydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	73.02	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Naloxone hydrochloride dihydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Naloxone hydrochloride dihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Naloxone hydrochloride di…	AP13501078IIN	22811	40	20160429
Audor Pharma	Naloxone hydrochloride di…	AP1547I022-1N	24707	40	20180629
Caelo	Naloxone hydrochloride di…	163577	23039	40	20170306*
Caelo	Naloxone hydrochloride di…	170441	23862	40	20170306*
Caelo	Naloxone hydrochloride di…	20001602	25447	40	20200604*
Euro OTC	Naloxone hydrochloride di…	2103008	25682	40	20210430*
Fagron	Naloxone hydrochloride di…	13D22-N07	20957	40	1402059
Fagron	Naloxone hydrochloride di…	13L12-B03	21271	40	20140113
Fagron	Naloxone hydrochloride di…	21J11-B10-216368	26175	40	20211118
Fagron	Naloxone hydrochloride di…	21J11-B10-216368	26175SI	40	20211118

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 400 spectra of 10 reference samples from the substance/substance group *Naloxone hydrochloride dihydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 562 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 370 spectra of 10 reference samples from the substance/substance group *Naloxone hydrochloride dihydrate*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Naloxone hydrochloride di…	15322517	22828	40
Caelo	Naloxone hydrochloride di…	190088	24537	40
Caelo	Naloxone hydrochloride di…	21000770009	26316	30
Caelo	Naloxone hydrochloride di…	22001102	27112	40
Euro OTC	Naloxone hydrochloride di…	2002011	25134	40
Euro OTC	Naloxone hydrochloride di…	2003062	25246	40
Euro OTC	Naloxone hydrochloride di…	2206005	26220	40
Euro OTC	Naloxone hydrochloride di…	2402028	27274	40
Caelo	Naloxone hydrochloride di…	21000770009	26316SI	20
Euro OTC	Naloxone hydrochloride di…	2206005	26220SI	40

- 201 714 spectra from a total of 4037 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 75 spectra from 27 *Apo-Ident* customers from 44 batches from the substance/substance group *Naloxone hydrochloride dihydrate*.

- Among them are spectra of independent samples from 43 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Naloxone hydrochloride di…	22001102004	1
	Naloxone hydrochloride di…	22001102008	1
Audor Pharma	Naloxone hydrochloride di…	AP13501078N	1
Audor Pharma	Naloxone hydrochloride di…	AP1547I022N	1
Caelo	Naloxone hydrochloride di…	15322501	1
Caelo	Naloxone hydrochloride di…	15322504	2
Caelo	Naloxone hydrochloride di…	15322517	1
Caelo	Naloxone hydrochloride di…	17044103	2
Caelo	Naloxone hydrochloride di…	18134202	3
Caelo	Naloxone hydrochloride di…	19008803	1
Caelo	Naloxone hydrochloride di…	20001602003	1
Caelo	Naloxone hydrochloride di…	2001602303	1
Caelo	Naloxone hydrochloride di…	20F15-F01-372581	2
Caesar & Loretz GmbH	Naloxone hydrochloride di…	19008803	2
Caesar & Loretz GmbH	Naloxone hydrochloride di…	20001602003	1
Euro OTC	Naloxone hydrochloride di…	2002011-01	1
Euro OTC	Naloxone hydrochloride di…	2003062-01	1
Fagron	Naloxone hydrochloride di…	11/23-N01	1
Fagron	Naloxone hydrochloride di…	12-00071	2
Fagron	Naloxone hydrochloride di…	12G19-N02	2
Fagron	Naloxone hydrochloride di…	12G19-NO2	1
Fagron	Naloxone hydrochloride di…	13-00660	1
Fagron	Naloxone hydrochloride di…	1350I078	1
Fagron	Naloxone hydrochloride di…	13L12-B03-289511	1
Fagron	Naloxone hydrochloride di…	14A28-B33-296076	1
Fagron	Naloxone hydrochloride di…	14F20-B02-296077	1
Fagron	Naloxone hydrochloride di…	15B06-B02-304420	2
Fagron	Naloxone hydrochloride di…	15B06-B02-304421	1
Fagron	Naloxone hydrochloride di…	15E28-B01-308324	5
Fagron	Naloxone hydrochloride di…	15H04-B09	3
Fagron	Naloxone hydrochloride di…	15H04-B09-314068	5
Fagron	Naloxone hydrochloride di…	15K11-B05_319571	1
Fagron	Naloxone hydrochloride di…	15K11-B05-319571	4
Fagron	Naloxone hydrochloride di…	18-00116	1
Fagron	Naloxone hydrochloride di…	18452304	1
Fagron	Naloxone hydrochloride di…	18C30-B04-349699	2
Fagron	Naloxone hydrochloride di…	18K20-B05-356947	4
Fagron	Naloxone hydrochloride di…	18K20-B05-356948	1
Fagron	Naloxone hydrochloride di…	19J22-F03	1
Fagron	Naloxone hydrochloride di…	19J22-F03-367715	2
Fagron	Naloxone hydrochloride di…	19J22-F03-367716	1
Fagron	Naloxone hydrochloride di…	19J22-F03-368419	1
Fagron	Naloxone hydrochloride di…	19J22-FO3-367715	1
Fagron	Naloxone hydrochloride di…	20F15-01-372577	1
Fagron	Naloxone hydrochloride di…	20F15-F01-372577	2
Fagron	Naloxone hydrochloride di…	20f15-f01-372581	2

- 235 992 spectra from 1515 *Apo-Ident* customers from a total of 49 214 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Naloxone hydrochloride dihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Naloxone hydrochloride dihydrate* and it was evaluated how many matches (positive) and rejections (negative) were

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	370	0	201 714
Type C	0	75	0	235 992

The substance/substance group *Naloxone hydrochloride dihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.3784 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 92.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20957	20957	0.00	89.68
21271	20957	11.09	86.01
22811	20957	21.25	92.34
23039	23039	0.00	93.62
23862	23862	0.00	92.62
24707	23039	20.77	96.04
25447	25447	0.00	81.46
25682	25682	0.00	88.69
26175	25682	22.31	86.36

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Naltrexone hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10006052-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Naltrexone hydrochloride; Naltrexoni hydrochloridum

Special notes

When selecting the *Naltrexone hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Naltrexone hydrochloride	5	1	0

Second-stage model

For differentiation of the substance/substance group *Naltrexone hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Naltrexone hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Naloxone hydrochloride dihydrate	68.69	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Naltrexone hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Naltrexone hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Naltrexone hydrochloride	2212013	26512	30	20221222*
Euro OTC	Naltrexone hydrochloride	2212013	26512SI	20	20221222*
Euro OTC	Naltrexone hydrochloride	2307013	26864	40	20230821*
Euro OTC	Naltrexone hydrochloride	2307013	26864SI	20	20230821*
Euro OTC	Naltrexone hydrochloride	2401025	27343	40	20240812*
Euro OTC	Naltrexone hydrochloride	2401025	27343SI	20	20240812*
Fagron	Naltrexone hydrochloride	22G14-B03-226174	26454	40	240401868
Fagron	Naltrexone hydrochloride	22G14-B03-226174	26454SI	20	240401868
Fagron	Naltrexone hydrochloride	24A19-B02-237101	27183	40	240704587

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 270 spectra of 9 reference samples from the substance/substance group *Naltrexone hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 692 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Naltrexone hydrochloride*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Naltrexone hydrochloride	23E16-B06-232752	26979	40

- 202 044 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Naltrexone hydrochloride*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Naltrexone hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Naltrexone hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	270	0	152 692
Type B	0	40	0	202 044
Type C	0	0	0	236 067

The substance/substance group *Naltrexone hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7778 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26454	26454	0.00	236.09
26512	26512	0.00	257.24
26864	26864	0.00	115.53
27183	27183	0.00	244.92
27343	27343	0.00	179.28

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Naphazoline hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20899-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Naphazoline hydrochloride; Naphazolini hydrochloridum

Special notes

When selecting the *Naphazoline hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Naphazoline hydrochloride	7	5	128

Second-stage model

For differentiation of the substance/substance group *Naphazoline hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Naphazoline hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Dexamphetamine sulfate	89.57	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Naphazoline hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Naphazoline hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Naphazoline hydrochloride	12375211	20899	40	20130108
Caelo	Naphazoline hydrochloride	12375211	21397	60	20130108
Caelo	Naphazoline hydrochloride	12375211	21398	60	20130108
Caelo	Naphazoline hydrochloride	181193	24498	40	20180504*
Euro OTC	Naphazoline hydrochloride	1407034-01	21623	60	AR-15-FG-007847-01
Euro OTC	Naphazoline hydrochloride	1506015	21859	60	20150727*
Euro OTC	Naphazoline hydrochloride	2003020	25260	40	20200706*
Euro OTC	Naphazoline hydrochloride	2008029	25304	40	20200908*
Fagron	Naphazoline hydrochloride	22K15-B02-223680	26449	40	20221129

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 440 spectra of 9 reference samples from the substance/substance group *Naphazoline hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 522 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Naphazoline hydrochloride*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Naphazoline hydrochloride	161741	24496	40
Caelo	Naphazoline hydrochloride	21000140004	26620	40
Euro OTC	Naphazoline hydrochloride	1607041	22753	40
Euro OTC	Naphazoline hydrochloride	1704005	23385	40
Euro OTC	Naphazoline hydrochloride	1903006	24613	40
Caelo	Naphazoline hydrochloride	21000140004	26620SI	20
Fagron	Naphazoline hydrochloride	22K15-B02-223680	26449SI†	20

- 201 844 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 357 spectra from 255 *Apo-Ident* customers from 137 batches from the substance/substance group *Naphazoline hydrochloride*.

- Among them are spectra of independent samples from 128 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Naphazoline hydrochloride	20E29-B01-215556	1
	Naphazoline hydrochloride	22K15-B02-223680	3
	Naphazoline hydrochloride	22K15-B02-228533	2
apo-ident	Naphazoline hydrochloride	200802901	1
Caelo	Naphazoline hydrochloride	11081107	2
Caelo	Naphazoline hydrochloride	1206037	1
Caelo	Naphazoline hydrochloride	1216203	1
Caelo	Naphazoline hydrochloride	12176203	2
Caelo	Naphazoline hydrochloride	12375203	1
Caelo	Naphazoline hydrochloride	12375211	1
Caelo	Naphazoline hydrochloride	1307020-02	1
Caelo	Naphazoline hydrochloride	140703402	1
Caelo	Naphazoline hydrochloride	1506015-02	2
Caelo	Naphazoline hydrochloride	1506015-2	1
Caelo	Naphazoline hydrochloride	15071404	1
Caelo	Naphazoline hydrochloride	15223301	2
Caelo	Naphazoline hydrochloride	15223303	1
Caelo	Naphazoline hydrochloride	15J05-B05/171025NHC	1
Caelo	Naphazoline hydrochloride	160704101	1
Caelo	Naphazoline hydrochloride	1607041-01	1
Caelo	Naphazoline hydrochloride	16174101	5
Caelo	Naphazoline hydrochloride	1704005-02	2
Caelo	Naphazoline hydrochloride	1704005-03	1
Caelo	Naphazoline hydrochloride	17C02-805	1
Caelo	Naphazoline hydrochloride	17C02-B05-341579	1
Caelo	Naphazoline hydrochloride	18119302	10
Caelo	Naphazoline hydrochloride	18119311	1
Caelo	Naphazoline hydrochloride	18D09-B08-350950	2
Caelo	Naphazoline hydrochloride	18D09-B08-352462	1
Caelo	Naphazoline hydrochloride	18D09-B08-354882	1
Caelo	Naphazoline hydrochloride	1900054002	1
Caelo	Naphazoline hydrochloride	19000544002	6
Caelo	Naphazoline hydrochloride	19000544006	3
Caelo	Naphazoline hydrochloride	20002382001	1
Caelo	Naphazoline hydrochloride	20002392001	1
Caelo	Naphazoline hydrochloride	20E29-B01-196687	1
Caelo	Naphazoline hydrochloride	21000140004	6
Caelo	Naphazoline hydrochloride	2275310	1
Caelo	Naphazoline hydrochloride	732570001	1
Caelo	Naphazoline hydrochloride	9285103	2
Caesar & Loretz GmbH Og	Naphazoline hydrochloride	20002392001	1
Caesar & Loretz GmbH/Gehe	Naphazoline hydrochloride	18119302	1
Caesar & Loretz GmbH	Naphazoline hydrochloride	18119302	1
Caesar & Loretz GmbH	Naphazoline hydrochloride	19000544002	3
Caesar & Loretz GmbH	Naphazoline hydrochloride	20002392001	1
Caesar & Loretz GmbH	Naphazoline hydrochloride	20002392004	2
Caesar & Loretz GmbH	Naphazoline hydrochloride	21000140004	1
Caesar & Loretz GmbH	Naphazoline hydrochloride	21001702002	1
Caesar & Loretz/Engel	Naphazoline hydrochloride	18119302	2
Caesar / Ebert	Naphazoline hydrochloride	17C02-B05-341579	1
Caleo /Herba	Naphazoline hydrochloride	9285103	1
Eurho/Phoenix	Naphazoline hydrochloride	4413I-01885	1
EuRho/Phönix	Naphazoline hydrochloride	1704005-03	1
EuRho	Naphazoline hydrochloride	1114I-001885	1
Euro OTC	Naphazoline hydrochloride	1103031-02	1
Euro OTC	Naphazoline hydrochloride	113031-01	1
Euro OTC	Naphazoline hydrochloride	1206037-01	3
Euro OTC	Naphazoline hydrochloride	1206037-02	4
Euro OTC	Naphazoline hydrochloride	1307020-03	2
Euro OTC	Naphazoline hydrochloride	14070034-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Naphazoline hydrochloride	1407034-01	2
Euro OTC	Naphazoline hydrochloride	1407034-02	4
Euro OTC	Naphazoline hydrochloride	1407034-03	1
Euro OTC	Naphazoline hydrochloride	1506015-01	3
Euro OTC	Naphazoline hydrochloride	150601502	1
Euro OTC	Naphazoline hydrochloride	1506015-02	6
Euro OTC	Naphazoline hydrochloride	1607041	1
Euro OTC	Naphazoline hydrochloride	1607041-01	7
Euro OTC	Naphazoline hydrochloride	1704005-02	5
Euro OTC	Naphazoline hydrochloride	1704005-03	2
Euro OTC	Naphazoline hydrochloride	19030006-01	1
Euro OTC	Naphazoline hydrochloride	190300601	1
Euro OTC	Naphazoline hydrochloride	1903006-01	5
Euro OTC	Naphazoline hydrochloride	2003020-01	2
Euro OTC	Naphazoline hydrochloride	2008029-01	3
Euro OTC	Naphazoline hydrochloride	616620001	1
Euro/Sanacorp	Naphazoline hydrochloride	1704005-03	1
Fagron	Naphazoline hydrochloride	11/05-N02	1
Fagron	Naphazoline hydrochloride	1196687	1
Fagron	Naphazoline hydrochloride	11I05-N02	2
Fagron	Naphazoline hydrochloride	11J13-N08	1
Fagron	Naphazoline hydrochloride	11K25-N03	2
Fagron	Naphazoline hydrochloride	12K29-N01	1
Fagron	Naphazoline hydrochloride	12K29-N01o256/310	1
Fagron	Naphazoline hydrochloride	13/03-B03	1
Fagron	Naphazoline hydrochloride	13/03-B03-295105	2
Fagron	Naphazoline hydrochloride	13/03-B03305291	1
Fagron	Naphazoline hydrochloride	13/03-B03-305291	1
Fagron	Naphazoline hydrochloride	1303-B03	1
Fagron	Naphazoline hydrochloride	1303B03305291	1
Fagron	Naphazoline hydrochloride	13103-803-305291	1
Fagron	Naphazoline hydrochloride	13A07-N06	4
Fagron	Naphazoline hydrochloride	13C11N07	1
Fagron	Naphazoline hydrochloride	13C11-N07	5
Fagron	Naphazoline hydrochloride	13C11-NO7	1
Fagron	Naphazoline hydrochloride	13I03-B03	2
Fagron	Naphazoline hydrochloride	13I03-B03-295105	3
Fagron	Naphazoline hydrochloride	13I03-B03-305291	2
Fagron	Naphazoline hydrochloride	13k27-n04	1
Fagron	Naphazoline hydrochloride	13K27-N04	13
Fagron	Naphazoline hydrochloride	13l03-B03-295105	3
Fagron	Naphazoline hydrochloride	15J05-B05	2
Fagron	Naphazoline hydrochloride	15J05-B05-322527	4
Fagron	Naphazoline hydrochloride	15J05B05326850	1
Fagron	Naphazoline hydrochloride	15J05-B05-326850	3
Fagron	Naphazoline hydrochloride	15J05-B05-330834	3
Fagron	Naphazoline hydrochloride	17c02-b05	1
Fagron	Naphazoline hydrochloride	17C02-B05	4
Fagron	Naphazoline hydrochloride	17C02-B05-332933	5
Fagron	Naphazoline hydrochloride	17C02-B05-335113	1
Fagron	Naphazoline hydrochloride	17c02-b05-335313	1
Fagron	Naphazoline hydrochloride	17C02-B05-335313	5
Fagron	Naphazoline hydrochloride	17C02-B05-341579	5
Fagron	Naphazoline hydrochloride	17C02-B05-343566	4
Fagron	Naphazoline hydrochloride	17C02-B05-346657	2
Fagron	Naphazoline hydrochloride	17C02-BO5-346657	1
Fagron	Naphazoline hydrochloride	1802201903	1
Fagron	Naphazoline hydrochloride	18D09	1
Fagron	Naphazoline hydrochloride	18D09-B08	2
Fagron	Naphazoline hydrochloride	18D09-B08-350950	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Naphazoline hydrochloride	18D09B08352462	1
Fagron	Naphazoline hydrochloride	18D09-B08-35462	1
Fagron	Naphazoline hydrochloride	18d09-b08-354882	1
Fagron	Naphazoline hydrochloride	18D09-B08-354882	7
Fagron	Naphazoline hydrochloride	18D09-B08-52462	1
Fagron	Naphazoline hydrochloride	18DO9-BO8-352462	1
Fagron	Naphazoline hydrochloride	19D03B02362717	1
Fagron	Naphazoline hydrochloride	19D03-B02-362717	5
Fagron	Naphazoline hydrochloride	20E29-801-196687	1
Fagron	Naphazoline hydrochloride	20E29-B01_196687	1
Fagron	Naphazoline hydrochloride	20e29b01196687	1
Fagron	Naphazoline hydrochloride	20E29B01196687	1
Fagron	Naphazoline hydrochloride	20E29-B01-196687	24
Fagron	Naphazoline hydrochloride	20E29-BO1-196687	1
Fagron	Naphazoline hydrochloride	20E801196687	1
Fagron	Naphazoline hydrochloride	2OE29B01196687	1
Fagron	Naphazoline hydrochloride	4309I-01885	1
Fagron	Naphazoline hydrochloride	4509E-01885	2
Fagron	Naphazoline hydrochloride	60494000113K27-N04	1
Fagron	Naphazoline hydrochloride	672530001	2
Fagron	Naphazoline hydrochloride	7001260012	1
Fagron	Naphazoline hydrochloride	700126-0012	1
Fagron	Naphazoline hydrochloride	706230001	3
Fagron	Naphazoline hydrochloride	708360002	1
Fagron	Naphazoline hydrochloride	9A09-N28	1
Fagron	Naphazoline hydrochloride	b01-1966807	1
Fagron	Naphazoline hydrochloride	B01-1966807	6
Fagron	Naphazoline hydrochloride	NPZ3020007	2
Fagron	Naphazoline hydrochloride	NPZ3O20007	2
Fargon/ Phönix	Naphazoline hydrochloride	20E29-B01-196687	1
Fargon/Apo.am Park	Naphazoline hydrochloride	539580002	1
Fargon/Noweda	Naphazoline hydrochloride	17C02-B05-346657	1
Fargon	Naphazoline hydrochloride	13/03-B03-295105	1
Fargron/Noweda	Naphazoline hydrochloride	20E29-B01-196687	1
Fragon GmbH/ Noweda	Naphazoline hydrochloride	15J05-B05-326850	1
Gatt-Koller	Naphazoline hydrochloride	1803834	1
Gehe/EuRho	Naphazoline hydrochloride	2008029-01	1
Gehe/EuRo	Naphazoline hydrochloride	1607041-01	1
Gehe	Naphazoline hydrochloride	17C02-B05-335313	1
Gehe	Naphazoline hydrochloride	19D03-B02-362717	2
Gehe	Naphazoline hydrochloride	20E29-B01-196687	1
Geilenkirchen	Naphazoline hydrochloride	18D09-B08-354882	1
Herberata Arzneimittel	Naphazoline hydrochloride	15223303I-02082016	1
Jenne	Naphazoline hydrochloride	2008029-01	1
LOBA / Gehe	Naphazoline hydrochloride	1903006-01	1
Loba / Gehe	Naphazoline hydrochloride	588710001	1
Nachprüfung	Naphazoline hydrochloride	3318E-1885	1
Noweda	Naphazoline hydrochloride	1704005-02	1
Noweda	Naphazoline hydrochloride	1903006-01	1
Noweda	Naphazoline hydrochloride	2003020-01	1
Noweda	Naphazoline hydrochloride	2008029-01	1
Noweda-Fragon	Naphazoline hydrochloride	1303B03305291	1
Otto Geilenkirchen	Naphazoline hydrochloride	22K15-B02-223680	1
Phoenix	Naphazoline hydrochloride	20E29-E01-196687	1
Phoenix	Naphazoline hydrochloride	22K15-B02-223680	1
Phonix	Naphazoline hydrochloride	1704005-02	1
Phönix	Naphazoline hydrochloride	1704005-02	2
Phönix	Naphazoline hydrochloride	586550002	1
Phönix	Naphazoline hydrochloride	B01-1966807	1

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 235 710 spectra from 1515 *Apo-Ident* customers from a total of 49 121 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Naphazoline hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Naphazoline hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	240	0	201 844
Type C	0	357	0	235 710

The substance/substance group *Naphazoline hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 98.3193 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20899	21859	16.01	157.87
21397	21859	4.29	164.62
21398	21859	4.45	160.45
21623	21623	0.00	161.84
21859	21859	0.00	163.67
24498	24498	0.00	154.89
25260	25260	0.00	133.55
25304	25304	0.00	131.09
26449	25260	6.96	135.48

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Naphazoline nitrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20501-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Naphazoline nitrate; Naphazolini nitras

Special notes

When selecting the *Naphazoline nitrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Naphazoline nitrate	7	3	27

Second-stage model

For differentiation of the substance/substance group *Naphazoline nitrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Naphazoline nitrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	110.60	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Naphazoline nitrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Naphazoline nitrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Naphazoline nitrate	1512033	22302	60	20160126*
Euro OTC	Naphazoline nitrate	1810016	24341	40	20181112*
Euro OTC	Naphazoline nitrate	1910029	24940	40	20191125*
Euro OTC	Naphazoline nitrate	2004011	25265	40	20200730*
Fagron	Naphazoline nitrate	12L10-N03	20846	40	20121217
Fagron	Naphazoline nitrate	12J08-B40-287904	21808	60	20131129
Fagron	Naphazoline nitrate	22E18-B01-221068	26453	40	20220705

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 320 spectra of 7 reference samples from the substance/substance group *Naphazoline nitrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 642 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Naphazoline nitrate*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Naphazoline nitrate	1512033-01	23275	40
Fagron	Naphazoline nitrate	16A14-B03-327343	23164	40
Fagron	Naphazoline nitrate	20D14-F02-370516	25490	40
Fagron	Naphazoline nitrate	22E18-B01-221068	26453SI†	20

- 201 944 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 42 spectra from 39 *Apo-Ident* customers from 28 batches from the substance/substance group *Naphazoline nitrate*.

- Among them are spectra of independent samples from 27 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
Alliance	Naphazoline nitrate	1810016-02	1
apomix	Naphazoline nitrate	2004011-01	1
Audor Pharma	Naphazoline nitrate	12I21-N05	1
Caelo	Naphazoline nitrate	18K30-B02-357305	1
eurho	Naphazoline nitrate	2004011-01	1
Euro OTC	Naphazoline nitrate	1810016-01	1
Euro OTC	Naphazoline nitrate	191002901	1
Euro OTC	Naphazoline nitrate	1910029-01	1
Euro OTC	Naphazoline nitrate	200401101	1
Euro OTC	Naphazoline nitrate	2004011-01	7
Euro OTC	Naphazoline nitrate	4011-0001	1
Euro OTC	Naphazoline nitrate	740530001	1
Euro OTC	Naphazoline nitrate	740530002	2
Fagron	Naphazoline nitrate	11I05-N03	1
Fagron	Naphazoline nitrate	12/21-N05	1
Fagron	Naphazoline nitrate	12J08-B40	1
Fagron	Naphazoline nitrate	12J08-B40-287904	1
Fagron	Naphazoline nitrate	12J08B40-294166	1
Fagron	Naphazoline nitrate	12J08-B40-294166	1
Fagron	Naphazoline nitrate	12j08-b40-303401	1
Fagron	Naphazoline nitrate	140214N	1
Fagron	Naphazoline nitrate	16A14-B03-322534	1
Fagron	Naphazoline nitrate	16A14-B03-327343	1
Fagron	Naphazoline nitrate	16A14-B03-333325	1
Fagron	Naphazoline nitrate	18K30-B02	1
Fagron	Naphazoline nitrate	18K30-B02-357305	2
Fagron	Naphazoline nitrate	20D14-F02-370516	3
Fagron	Naphazoline nitrate	21021304	1
Fagron	Naphazoline nitrate	2717M-07042	1
Fagron	Naphazoline nitrate	740530001	1
Fagron	Naphazoline nitrate	D14F02-370516	1
Noweda	Naphazoline nitrate	2004011-03	1

- 236 025 spectra from 1515 *Apo-Ident* customers from a total of 49 230 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Naphazoline nitrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Naphazoline nitrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	140	0	201 944
Type C	0	40	2	236 025

The substance/substance group *Naphazoline nitrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	95.2381 % (> 88.0952 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20846	22302	9.73	231.05
21808	22302	6.68	234.90
22302	22302	0.00	239.34
24341	24341	0.00	240.11
24940	24940	0.00	236.20
25265	25265	0.00	232.01
26453	24940	9.27	238.35

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Naproxen**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	22316-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Naproxen; Naproxenum

Special notes

When selecting the *Naproxen* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Naproxen	5	2	3

Second-stage model

For differentiation of the substance/substance group *Naproxen* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Naproxen* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	99.84	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Naproxen* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Naproxen*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Naproxen	15F18-B03-309492	22316	45	AR-16-FG-008486-02
Fagron	Naproxen	15F18-B03-315691	22327	45	20150703
Fagron	Naproxen	16B04-B09-326261	23105	40	20160229
Fagron	Naproxen	22H17-B03-227263	26542	40	20221004
Fagron	Naproxen	22H17-B03-227263	26542SI	20	20221004
Fagron	Naproxen	23F19-B01-236106	27188	40	20230711
Fagron	Naproxen	23F19-B01-236106	27188SI	20	20230711

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 250 spectra of 7 reference samples from the substance/substance group *Naproxen*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 712 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 3 reference samples from the substance/substance group *Naproxen*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Naproxen	17C10-B03-336472	23763	40
Fagron	Naproxen	21F15-B16-213613	25909	40
Fagron	Naproxen	21F15-B16-213613	25909SI	10

- 201 994 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 27 spectra from 6 *Apo-Ident* customers from 3 batches from the substance/substance group *Naproxen*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Fagron	Naproxen	13E31-B40-287536	2
Fagron	Naproxen	16B04-B09-321569	24
Fagron	Naproxen	17C10-B03-336472	1

- 236 040 spectra from 1515 *Apo-Ident* customers from a total of 49 255 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Naproxen* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Naproxen* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	250	0	152 712
Type B	0	90	0	201 994
Type C	0	27	0	236 040

The substance/substance group *Naproxen* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 93.3333 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 77.7778 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22316	22316	0.00	156.02
22327	22316	2.02	156.56
23105	22316	5.59	158.79
26542	22316	7.35	156.24
27188	22316	7.61	159.21

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Neomycin sulfate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20544-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Neomycin sulfate; Neomycin sulphate; Neomycini sulfas

Special notes

When selecting the *Neomycin sulfate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Neomycin sulfate	12	5	223

Second-stage model

For differentiation of the substance/substance group *Neomycin sulfate* the following second-stage model is used:

- Submodel 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Neomycin sulfate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Tobramycin sulfate	34.78	29.19
Sodium cromoglicate	55.07	–
⋮	⋮	⋮
Mg-Ca-K colamine phosphate	>50	59.93
Riboflavin sodium phosphate hydrate	>50	63.65
Zinc gluconate	>50	91.37
Gentamicin sulfate	>50	115.97
Carbomers	>50	116.21
Magnesium citrate	>50	121.55
Sodium tetraborate	>50	403.69
Finasteride	>50	1490.52

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Neomycin sulfate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Neomycin sulfate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Neomycin sulfate	13062923	21814	60	AR-15-FG-016581-01
Caelo	Neomycin sulfate	13062923	22276	45	20130315
Caelo	Neomycin sulfate	161650	23856	30	20160629*
Caelo	Neomycin sulfate	20002248	25643	40	20200923*
Caelo	Neomycin sulfate	24000508	27222	40	20240416*
Euro OTC	Neomycin sulfate	1303033-03	21771	60	AR-15-FG-016582-01
Euro OTC	Neomycin sulfate	1601046	22381	45	20160212*
Fagron	Neomycin sulfate	14C27-B05-302516	21894	60	1604527
Fagron	Neomycin sulfate	14C27-B05-302517	21961	60	20140418
Fagron	Neomycin sulfate	19G23-B03-364716	25185	40	20191007
Fagron	Neomycin sulfate	22E11-B04-224107	26286	40	20220627

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Neomycin sulfate	23C10-B04-219531	26664	40	20230310
Fagron	Neomycin sulfate	23C10-B04-219531	26664SI	20	20230310
Fagron	Neomycin sulfate	23G20-B10-233758	27052	40	20230803

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 620 spectra of 14 reference samples from the substance/substance group *Neomycin sulfate*. These samples are listed above in the *calibration samples* section. The reference samples come from 12 different batches.

- 152 342 spectra from a total of 2830 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Neomycin sulfate*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Neomycin sulfate	15237602	22389	40
Caelo	Neomycin sulfate	23000856	26894	40
Euro OTC	Neomycin sulfate	1802005	23952	40
Euro OTC	Neomycin sulfate	1903022	24642	40
Euro OTC	Neomycin sulfate	2003021	25280	40
Caelo	Neomycin sulfate	23000856	26894SI	20
Fagron	Neomycin sulfate	22E11-B04-224107	26286SI†	20

- 201 844 spectra from a total of 4039 batches from further 838 substances. These spectra were

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1215 spectra from 539 *Apo-Ident* customers from 239 batches from the substance/substance group *Neomycin sulfate*.
- Among them are spectra of independent samples from 223 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Neomycin sulfate	1303033-03	1
	Neomycin sulfate	13G09-N07	1
	Neomycin sulfate	2100321600	1
	Neomycin sulfate	23000856006	3
	Neomycin sulfate	23000856007	5
	Neomycin sulfate	23C10-B04-219532	3
	Neomycin sulfate	23C10-B04-219532	1
	Neomycin sulfate	23D14-B03-232374	5
	Neomycin sulfate	24000508004	1
	Neomycin sulfate	24000508005	1
	Neomycin sulfate	B03_2323704	1
	Neomycin sulfate	GY9146	1
AHD/Euro	Neomycin sulfate	160104602	1
AHD/Euro	Neomycin sulfate	1802005	1
AHD	Neomycin sulfate	11/19-N14	1
AHD	Neomycin sulfate	14A31-B02-294698	2
AHD	Neomycin sulfate	1802005-01	2
Alliance Health 13.01.204	Neomycin sulfate	1303033-01	2
Alliance Healthcare	Neomycin sulfate	1102043-03	1
Alliance	Neomycin sulfate	1802005-01	1
Alliance	Neomycin sulfate	2003021-02	1
ApBetrO/Noweda	Neomycin sulfate	200302-02	1
apo-ident.;4,45EUR; Sa...	Neomycin sulfate	1601046-01	1
Ashland/Sanacorp	Neomycin sulfate	1303033-02	1
aurica/phoenix	Neomycin sulfate	1102043-02	1
Caelo	Neomycin sulfate	10157505	5
Caelo	Neomycin sulfate	10206300	1
Caelo	Neomycin sulfate	1102043-02	1
Caelo	Neomycin sulfate	11C21-N10	1
Caelo	Neomycin sulfate	12175401	4
Caelo	Neomycin sulfate	12276405	1
Caelo	Neomycin sulfate	12276410	2
Caelo	Neomycin sulfate	1303033-02	1
Caelo	Neomycin sulfate	130303303	3
Caelo	Neomycin sulfate	1303033-03	3
Caelo	Neomycin sulfate	13062905	2
Caelo	Neomycin sulfate	13062908	1
Caelo	Neomycin sulfate	13062921	1
Caelo	Neomycin sulfate	13062922	1
Caelo	Neomycin sulfate	13062923	6
Caelo	Neomycin sulfate	13D10N05	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Neomycin sulfate	13G09-N07	1
Caelo	Neomycin sulfate	14A31-B02-294696	1
Caelo	Neomycin sulfate	1502004-01	1
Caelo	Neomycin sulfate	1502004-03	2
Caelo	Neomycin sulfate	15237602	7
Caelo	Neomycin sulfate	15298902	2
Caelo	Neomycin sulfate	15J09-B04-314015	1
Caelo	Neomycin sulfate	15J27-B07-321372	1
Caelo	Neomycin sulfate	1601046	1
Caelo	Neomycin sulfate	1601046-01	3
Caelo	Neomycin sulfate	1601046-02	2
Caelo	Neomycin sulfate	16122601	3
Caelo	Neomycin sulfate	16122611	2
Caelo	Neomycin sulfate	16122612	8
Caelo	Neomycin sulfate	16122617	1
Caelo	Neomycin sulfate	16122618	1
Caelo	Neomycin sulfate	16122623	1
Caelo	Neomycin sulfate	16165004	4
Caelo	Neomycin sulfate	16165006	3
Caelo	Neomycin sulfate	16165008	2
Caelo	Neomycin sulfate	16165014	1
Caelo	Neomycin sulfate	161650145351	1
Caelo	Neomycin sulfate	16165015	1
Caelo	Neomycin sulfate	16165016	15
Caelo	Neomycin sulfate	16165017	2
Caelo	Neomycin sulfate	16165018	7
Caelo	Neomycin sulfate	16B10-B50-328165	3
Caelo	Neomycin sulfate	17F12-B04-340237	2
Caelo	Neomycin sulfate	18018704	7
Caelo	Neomycin sulfate	180200501	1
Caelo	Neomycin sulfate	1802005-01	9
Caelo	Neomycin sulfate	18161303	14
Caelo	Neomycin sulfate	18161304	4
Caelo	Neomycin sulfate	18161305	6
Caelo	Neomycin sulfate	18161307	17
Caelo	Neomycin sulfate	18161309	1
Caelo	Neomycin sulfate	18161310	8
Caelo	Neomycin sulfate	18A25-B05-346135	1
Caelo	Neomycin sulfate	18A25-B05-346138	1
Caelo	Neomycin sulfate	18G28B05352957	1
Caelo	Neomycin sulfate	18G28B05354472	1
Caelo	Neomycin sulfate	191849001	6
Caelo	Neomycin sulfate	191849003	8
Caelo	Neomycin sulfate	19184903	18
Caelo	Neomycin sulfate	20000391004	6
Caelo	Neomycin sulfate	200003914004	1
Caelo	Neomycin sulfate	20004305001	11
Caelo	Neomycin sulfate	20004305005	9
Caelo	Neomycin sulfate	20004305006	4
Caelo	Neomycin sulfate	2003021-02	2
Caelo	Neomycin sulfate	20E13-F-03	1
Caelo	Neomycin sulfate	21003216005	14
Caelo	Neomycin sulfate	21003216006	3
Caelo	Neomycin sulfate	21003216022	2
Caelo	Neomycin sulfate	21003216023	1
Caelo	Neomycin sulfate	21003216025	1
Caelo	Neomycin sulfate	21003216027	5
Caelo	Neomycin sulfate	2120520043055	1
Caelo	Neomycin sulfate	23000856007	1
Caelo	Neomycin sulfate	24111203	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Neomycin sulfate	3345	1
Caelo	Neomycin sulfate	5/AKD35	1
Caelo	Neomycin sulfate	5/AKD36	1
Caelo	Neomycin sulfate	563313062905	1
Caelo	Neomycin sulfate	8718	1
Caelo	Neomycin sulfate	9051402	1
Caelo	Neomycin sulfate	9105316	1
Caelo	Neomycin sulfate	L34419	1
Caelo	Neomycin sulfate	N05780	1
Caesar & Loretz GmbH...	Neomycin sulfate	11/19-N14	1
Caesar & Loretz GmbH...	Neomycin sulfate	19184903	1
Caesar & Loretz GmbH...	Neomycin sulfate	20004305005	1
Caesar & Loretz GmbH...	Neomycin sulfate	20004305005	1
Caesar & Loretz GmbH/Gehe	Neomycin sulfate	21003216026	1
Caesar & Loretz GmbH...	Neomycin sulfate	21003216006	3
Caesar & Loretz GmbH...	Neomycin sulfate	19184903	1
Caesar & Loretz GmbH...	Neomycin sulfate	18161310	2
Caesar & Loretz GmbH...	Neomycin sulfate	21003216005	1
Caesar & Loretz GmbH	Neomycin sulfate	18018704	2
Caesar & Loretz GmbH	Neomycin sulfate	18161305	2
Caesar & Loretz GmbH	Neomycin sulfate	18161307	7
Caesar & Loretz GmbH	Neomycin sulfate	191849001	4
Caesar & Loretz GmbH	Neomycin sulfate	19184903	10
Caesar & Loretz GmbH	Neomycin sulfate	20000391004	1
Caesar & Loretz GmbH	Neomycin sulfate	20004305001	3
Caesar & Loretz GmbH	Neomycin sulfate	20004305005	6
Caesar & Loretz GmbH	Neomycin sulfate	20004305006	2
Caesar & Loretz GmbH	Neomycin sulfate	21003216005	7
Caesar & Loretz GmbH	Neomycin sulfate	21003216022	1
Caesar & Loretz GmbH	Neomycin sulfate	21003216026	2
Caesar Loretz	Neomycin sulfate	19184903	1
Caesar&Loretz GmbH,1...	Neomycin sulfate	16122612	1
Caesar&loretz,AHC,05...	Neomycin sulfate	15237602	1
caesar&loretz,AHC,7.3.16	Neomycin sulfate	13062923	1
Caesar&loretz,Phoenix	Neomycin sulfate	12C13-N04	1
Caesar&Loretz/Noweda	Neomycin sulfate	15298904	1
Cealo/AHD	Neomycin sulfate	15J09-B04-314017	1
Cealo	Neomycin sulfate		1
cealo	Neomycin sulfate	1502004-03	1
Ebert & Jacobi	Neomycin sulfate	1601046-01	1
Eur Rho Gehe	Neomycin sulfate	2003021-01	1
EuRho / Fiebig	Neomycin sulfate	2003021-02	1
EuRho/Sanacorp	Neomycin sulfate	1102043-03	1
EuRho/Sanacorp	Neomycin sulfate	1502004-01	2
EuRho	Neomycin sulfate	1102043-02	1
EuRho	Neomycin sulfate	1601046-01	1
Eurho	Neomycin sulfate	1601046-02	1
EuRho	Neomycin sulfate	1802005-01	2
euRho	Neomycin sulfate	1903022-01	1
EuRho	Neomycin sulfate	2003021-01	2
EuRho	Neomycin sulfate	2003021-02	1
Euro OTC	Neomycin sulfate	1102043	2
Euro OTC	Neomycin sulfate	1102043-01	3
Euro OTC	Neomycin sulfate	1102043-02	7
Euro OTC	Neomycin sulfate	1102043-03	4
Euro OTC	Neomycin sulfate	1303001-03	1
Euro OTC	Neomycin sulfate	1303033-01	10
Euro OTC	Neomycin sulfate	1303033-02	15
Euro OTC	Neomycin sulfate	1303033-03	17
Euro OTC	Neomycin sulfate	1502004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Neomycin sulfate	1502004-01	19
Euro OTC	Neomycin sulfate	1502004-02	4
Euro OTC	Neomycin sulfate	1502004-03	23
Euro OTC	Neomycin sulfate	151116N	1
Euro OTC	Neomycin sulfate	1601042	1
Euro OTC	Neomycin sulfate	1601045-01	2
Euro OTC	Neomycin sulfate	1601046	1
Euro OTC	Neomycin sulfate	160104601	3
Euro OTC	Neomycin sulfate	1601046-01	37
Euro OTC	Neomycin sulfate	1601046-02	41
Euro OTC	Neomycin sulfate	1601046-1	1
Euro OTC	Neomycin sulfate	160146-02	1
Euro OTC	Neomycin sulfate	16019046-01	1
Euro OTC	Neomycin sulfate	18020005-01	2
Euro OTC	Neomycin sulfate	180200501	2
Euro OTC	Neomycin sulfate	1802005-01	136
Euro OTC	Neomycin sulfate	1802-005-01	1
Euro OTC	Neomycin sulfate	180205-01	1
Euro OTC	Neomycin sulfate	1802095	1
Euro OTC	Neomycin sulfate	190302-01	1
Euro OTC	Neomycin sulfate	1903022	3
Euro OTC	Neomycin sulfate	1903022-01	18
Euro OTC	Neomycin sulfate	191001209	1
Euro OTC	Neomycin sulfate	2003021	3
Euro OTC	Neomycin sulfate	200302101	1
Euro OTC	Neomycin sulfate	2003021-01	33
Euro OTC	Neomycin sulfate	200302102	1
Euro OTC	Neomycin sulfate	2003021-02	63
Euro OTC	Neomycin sulfate	3021-012	1
Euro OTC	Neomycin sulfate	3519A-01926	1
Euro OTC	Neomycin sulfate	G73890	1
Euro OTC	Neomycin sulfate	L34419	4
Euro OTC	Neomycin sulfate	N05780	1
Euro OTC	Neomycin sulfate	w13203	1
Euro OTC	Neomycin sulfate	W13203	2
euro//Noweda	Neomycin sulfate	1601046-02	1
Euro/Phönix	Neomycin sulfate	1502004-01	1
Euro/Phönix	Neomycin sulfate	1502004-03	1
Euro/Phönix	Neomycin sulfate	2003021-01	1
Euro/Sanacorp	Neomycin sulfate	1601046-02	1
Euro/Sanacorp	Neomycin sulfate	1661046-02	2
Euro/Sanacorp	Neomycin sulfate	1802005-01	2
Euro/Sanacorp	Neomycin sulfate	2003021-01	1
euro	Neomycin sulfate	1502004-02	2
Euroo/Noweda	Neomycin sulfate	2003021-01	1
Eurp	Neomycin sulfate	2003021	1
Fagron	Neomycin sulfate	100810-112-91	1
Fagron	Neomycin sulfate	10121-N01	1
Fagron	Neomycin sulfate	11/19-N14	4
Fagron	Neomycin sulfate	116M-01926	1
Fagron	Neomycin sulfate	11C21-N10	3
Fagron	Neomycin sulfate	12C13-N04	4
Fagron	Neomycin sulfate	12H23-N04	6
Fagron	Neomycin sulfate	12I19-N14	1
Fagron	Neomycin sulfate	13D10-N05	5
Fagron	Neomycin sulfate	13D10-NO5	1
Fagron	Neomycin sulfate	13G09-N06	1
Fagron	Neomycin sulfate	13G09N07	2
Fagron	Neomycin sulfate	13G09-N07	16
Fagron	Neomycin sulfate	13G09-N070129/340	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Neomycin sulfate	13K15-B33-288069	3
Fagron	Neomycin sulfate	13K15-B33-288073	1
Fagron	Neomycin sulfate	14A31B02	2
Fagron	Neomycin sulfate	14A31-B02	2
Fagron	Neomycin sulfate	14A31B02294696	1
Fagron	Neomycin sulfate	14A31-B02-294696	5
Fagron	Neomycin sulfate	14A31-B02-294697	1
Fagron	Neomycin sulfate	14A31-B02-294698	1
Fagron	Neomycin sulfate	14A31-B02-296724	1
Fagron	Neomycin sulfate	14A31-B02-302519	5
Fagron	Neomycin sulfate	14C27-B05	1
Fagron	Neomycin sulfate	14c27-B05-302516	1
Fagron	Neomycin sulfate	14C27-B05-302516	2
Fagron	Neomycin sulfate	14C27-B05-302517	1
Fagron	Neomycin sulfate	15/27-B07-321372	2
Fagron	Neomycin sulfate	1502004-01	2
Fagron	Neomycin sulfate	1502004-03	1
Fagron	Neomycin sulfate	15i09-B04-314015	1
Fagron	Neomycin sulfate	15J09-B04	1
Fagron	Neomycin sulfate	15j09-b04-314015	1
Fagron	Neomycin sulfate	15J09-B04314015	1
Fagron	Neomycin sulfate	15J09-B04-314015	5
Fagron	Neomycin sulfate	15J09-B04-314017	5
Fagron	Neomycin sulfate	15J27-B07	1
Fagron	Neomycin sulfate	15J27-B07-321372	2
Fagron	Neomycin sulfate	15JO9-BO4-314017	1
Fagron	Neomycin sulfate	16A20-B01-327433	1
Fagron	Neomycin sulfate	16A20-B10	2
Fagron	Neomycin sulfate	16A20-B10-324346	2
Fagron	Neomycin sulfate	16A20-B10-327433	2
Fagron	Neomycin sulfate	16b10-b50	1
Fagron	Neomycin sulfate	16B10-B50	3
Fagron	Neomycin sulfate	16B10-B50-328165	10
Fagron	Neomycin sulfate	16B28-B05-352957	1
Fagron	Neomycin sulfate	17B14-B08	1
Fagron	Neomycin sulfate	17B14-B08-334000	3
Fagron	Neomycin sulfate	17F12-804	1
Fagron	Neomycin sulfate	17F12-B04	1
Fagron	Neomycin sulfate	17f12-b04-340237	1
Fagron	Neomycin sulfate	17F12-B04-340237	1
Fagron	Neomycin sulfate	17G05-B04	1
Fagron	Neomycin sulfate	180200501	1
Fagron	Neomycin sulfate	1802005-01	6
Fagron	Neomycin sulfate	183360-0009	1
Fagron	Neomycin sulfate	18A25-B05-346136	1
Fagron	Neomycin sulfate	18A25-B05-346138	4
Fagron	Neomycin sulfate	18A25-B-05-346138	1
Fagron	Neomycin sulfate	18G28B05	1
Fagron	Neomycin sulfate	18G28-B05	3
Fagron	Neomycin sulfate	18g28-b05-352953	1
Fagron	Neomycin sulfate	18G28-B05-352953	5
Fagron	Neomycin sulfate	18G28-B05-352957	4
Fagron	Neomycin sulfate	18G28-B05-354472	7
Fagron	Neomycin sulfate	19G23-B03	1
Fagron	Neomycin sulfate	19G23-B03-364716	3
Fagron	Neomycin sulfate	19G23-B03-364717	1
Fagron	Neomycin sulfate	19G23-B03-364720	4
Fagron	Neomycin sulfate	19G23-BO3-364717	1
Fagron	Neomycin sulfate	19G23-BO3-364720	1
Fagron	Neomycin sulfate	19i23-b04-195473	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Neomycin sulfate	20A29-F01	1
Fagron	Neomycin sulfate	20A29-F01-370834	2
Fagron	Neomycin sulfate	20A29-F01-370836	6
Fagron	Neomycin sulfate	20A29F01370841	1
Fagron	Neomycin sulfate	20A29-F01-370841	3
Fagron	Neomycin sulfate	20A29-F01-370842	1
Fagron	Neomycin sulfate	20A29-F01-370836	2
Fagron	Neomycin sulfate	20D08-B07-200574	1
Fagron	Neomycin sulfate	20do8-b07-200574	1
Fagron	Neomycin sulfate	20do8-b07-201750	1
Fagron	Neomycin sulfate	20E13-F03-371373	1
Fagron	Neomycin sulfate	21D30-F06	2
Fagron	Neomycin sulfate	21D30-F06-378610	2
Fagron	Neomycin sulfate	21D30-F06-378614	9
Fagron	Neomycin sulfate	21D3O-F06-378614	1
Fagron	Neomycin sulfate	22E12-B10-224471	1
Fagron	Neomycin sulfate	23A09-B07-229452	1
Fagron	Neomycin sulfate	23C10-B04-219531	1
Fagron	Neomycin sulfate	352954	1
Fagron	Neomycin sulfate	4312I-01926	1
Fagron	Neomycin sulfate	b03-364717	1
Fagron	Neomycin sulfate	F08469	1
Fagron	Neomycin sulfate	FO8469	1
Fagron	Neomycin sulfate	M71862	2
Fagron	Neomycin sulfate	NMZ11006K	1
Fagron	Neomycin sulfate	X51344	1
Fargon / AHD	Neomycin sulfate	18G28-B05-354472	1
Fargon	Neomycin sulfate	15j27-b07-321372	1
fargron	Neomycin sulfate	14A31-B02-294698	1
Fiebig	Neomycin sulfate	1502004-03	2
Fragon/Phoenix	Neomycin sulfate	15J09-B04_322943	1
Gehe 23.11.18	Neomycin sulfate	1802005-01	1
Gehe Apo-ident	Neomycin sulfate	200302102	2
GEHE	Neomycin sulfate	1502001-03	1
Gehe	Neomycin sulfate	1601046-01	1
Gehe	Neomycin sulfate	1601046-02	1
GEHE	Neomycin sulfate	160104602	1
Gehe	Neomycin sulfate	1802005-01	1
GEHE	Neomycin sulfate	1802005-01	1
gehe	Neomycin sulfate	183360-0009	1
Gehe	Neomycin sulfate	183360-0009	1
Gehe	Neomycin sulfate	194A-01926	1
Gehe	Neomycin sulfate	2003021-02	2
Gehe	Neomycin sulfate	2100321606	1
Gehe	Neomycin sulfate	23D14-B03-232374	1
Geibo/EuRho	Neomycin sulfate	180200501	1
Geibo/EuRho	Neomycin sulfate	1802005-01	1
Hageda	Neomycin sulfate	1802005-01	1
HenryLamotte	Neomycin sulfate	1502004-01	1
Jenne	Neomycin sulfate	15237602	1
Jenne	Neomycin sulfate	20004305006	1
Jenne	Neomycin sulfate	GY9146	1
Kehr	Neomycin sulfate	1601046-02	1
Land/Phönix	Neomycin sulfate	13062905	2
Nachprüfung	Neomycin sulfate	2082019-7	1
Noweda/Euro	Neomycin sulfate		1
Noweda	Neomycin sulfate	1102043-02	1
Noweda	Neomycin sulfate	15298902	1
Noweda	Neomycin sulfate	160104601	1
Noweda	Neomycin sulfate	1601046-02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Neomycin sulfate	16165016	1
Noweda	Neomycin sulfate	1802005-01	3
Noweda	Neomycin sulfate	191849001	1
Noweda	Neomycin sulfate	20004305001	1
Noweda	Neomycin sulfate	20A29-F01-370841	1
Noweda	Neomycin sulfate	21003216005	2
Noweda	Neomycin sulfate	23C10-B04-219531	1
Noweda	Neomycin sulfate	23D14-B03-232374	2
Pfizer USA / Phönix	Neomycin sulfate	1303033-02	1
Pfizer USA/ Phönix	Neomycin sulfate	DC3552	1
Pfizer USA/Phoenix	Neomycin sulfate	2003021-21	1
Pfizer usa	Neomycin sulfate	160104601	1
Pfizer USA	Neomycin sulfate	2003021	1
Pfizer USA	Neomycin sulfate	DC3552	1
Pfizer/Euro OCT Pharma	Neomycin sulfate	1102043-02	2
Pfizer/Noweda	Neomycin sulfate	W13203	1
Ph/Euro	Neomycin sulfate	18020501	1
Pharmacia & Upjohn C...	Neomycin sulfate	16165017	1
Pharmacia & Upjohn C...	Neomycin sulfate	16122623	1
phnoix	Neomycin sulfate	130303301	1
phoenix 13.11.14	Neomycin sulfate	1303033-03	1
Phoenix	Neomycin sulfate	1601046-02	2
Phoenix	Neomycin sulfate	2003021-01	1
Phoenix	Neomycin sulfate	23000856007	1
Phoenix	Neomycin sulfate	2400508005	1
Phönix Euro 23.6.21	Neomycin sulfate	2003021-01	1
Phönix	Neomycin sulfate	13D10-N05	1
Phönix	Neomycin sulfate	1601046-02	1
Phönix	Neomycin sulfate	1802005-01	3
Phönix	Neomycin sulfate	18A25B05-346138	1
Sanacop/Pharma	Neomycin sulfate	15J27B07-321372	1
Sanacorp 05.07.2019 5,90EUR	Neomycin sulfate	18G28-B05-354472	1
Sanacorp/EuRho	Neomycin sulfate	1601046-01	1
Sanacorp	Neomycin sulfate	15298902	1
Sanacorp	Neomycin sulfate	16165016	1
Sanacorp	Neomycin sulfate	180200501	1
Sanacorp	Neomycin sulfate	2003021-02	1
Sanacorp	Neomycin sulfate	23C10-B04-219532	1
Sanacorp	Neomycin sulfate	23D14-B03-232374	2
Sichuan Long March P...	Neomycin sulfate	SC-NM-20180109	1
Sichuan Long March P...	Neomycin sulfate	SC-NM-20190123	3
Sichuan/Noweda	Neomycin sulfate	SC-NM-20200410	1
siehe WE-Prüfprotokoll	Neomycin sulfate	19/12	1
Taoasis/Phoenix	Neomycin sulfate	1502004-01	1
VDL;24.6.14; 3,55EUR	Neomycin sulfate	1303033-02	2
VDL;9.12;3,55;	Neomycin sulfate	1303033-03	1

- 234 852 spectra from 1515 *Apo-Ident* customers from a total of 49 022 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Neomycin sulfate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Neomycin sulfate* and it was evaluated

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	620	0	152 342
Type B	0	240	0	201 844
Type C	0	1208	7	234 852

The substance/substance group *Neomycin sulfate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0323 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	99.4239 % (> 99.1770 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21771	21771	0.00	113.96
21814	21814	0.00	121.41
21894	21894	0.00	91.71
21961	21814	19.92	119.25
22276	21814	3.44	121.12
22381	22381	0.00	130.86
23856	23856	0.00	76.22
25185	22381	8.40	139.76
25643	25643	0.00	112.36
26286	21771	10.62	118.13
26664	22381	15.16	141.16
27052	22381	28.14	95.61
27222	27222	0.00	92.18

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Neostigmine bromide**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20717-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Neostigmine bromide; Neostigmini bromidum

Special notes

When selecting the *Neostigmine bromide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Neostigmine bromide	5	3	12

Second-stage model

For differentiation of the substance/substance group *Neostigmine bromide* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Neostigmine bromide* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Dequalinium chloride	113.63	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Neostigmine bromide* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Neostigmine bromide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Neostigmine bromide	10144105	20717	40	20100616
Caelo	Neostigmine bromide	12172304	20990	40	1403163
Caelo	Neostigmine bromide	14256802	21816	60	AR-15-FG-014460-01
Caelo	Neostigmine bromide	14256802	21816SI	60	AR-15-FG-014460-01
Caelo	Neostigmine bromide	15228101	21919	60	20151002
Caelo	Neostigmine bromide	15228101	21919SI	60	20151002
Caelo	Neostigmine bromide	193083001	25390	40	20191213

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 7 reference samples from the substance/substance group *Neostigmine bromide*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 602 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 280 spectra of 7 reference samples from the substance/substance group *Neostigmine bromide*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Neostigmine bromide	171319	23369	40
Caelo	Neostigmine bromide	17131901	23373	40
Caelo	Neostigmine bromide	22000195	26012	40
Caelo	Neostigmine bromide	171319	23369SI	40
Caelo	Neostigmine bromide	17131901	23373SI	40
Caelo	Neostigmine bromide	193083001	25390SI†	40
Caelo	Neostigmine bromide	22000195	26012SI	40

- 201 804 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 43 spectra from 18 *Apo-Ident* customers from 16 batches from the substance/substance group *Neostigmine bromide*.
- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Neostigmine bromide	12172301	1
Caelo	Neostigmine bromide	12172304	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Neostigmine bromide	13177201	1
Caelo	Neostigmine bromide	13177203	2
Caelo	Neostigmine bromide	13177206	6
Caelo	Neostigmine bromide	131772303A	1
Caelo	Neostigmine bromide	131772303B	1
Caelo	Neostigmine bromide	14256802	3
Caelo	Neostigmine bromide	15228101	3
Caelo	Neostigmine bromide	15228103	2
Caelo	Neostigmine bromide	17131901	4
Caelo	Neostigmine bromide	17131903	5
Caelo	Neostigmine bromide	18024902	2
Caelo	Neostigmine bromide	193083001	3
Caelo	Neostigmine bromide	20003839001	1
Caesar & Loretz GmbH	Neostigmine bromide	18024902	2
Gehe	Neostigmine bromide	12172301	1
Gehe	Neostigmine bromide	12172307	1
Gehe	Neostigmine bromide	13177201	1
Hetterich/Noewda	Neostigmine bromide	17131901	1
Sanacorp	Neostigmine bromide	18024902	1

- 236 024 spectra from 1515 *Apo-Ident* customers from a total of 49 242 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Neostigmine bromide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Neostigmine bromide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	280	0	201 804
Type C	0	43	0	236 024

The substance/substance group *Neostigmine bromide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.8571 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 86.0465 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20717	20990	7.00	154.76
20990	20990	0.00	156.82
21816	21816	0.00	185.85
21919	21816	28.00	174.28
25390	20990	37.69	167.62

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Nicotinamide**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20335-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Nicotinamide; Nicotinamidum

Special notes

When selecting the *Nicotinamide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Nicotinamide	9	13	54

Second-stage model

For differentiation of the substance/substance group *Nicotinamide* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Nicotinamide* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	104.37	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Nicotinamide* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Nicotinamide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Nicotinamide	13097506	21364	40	20130416
Caelo	Nicotinamide	163048	23038	40	20161123*
Caelo	Nicotinamide	163048	23050	40	20161123*
Euro OTC	Nicotinamide	1310025-01	21643	60	20131121
Euro OTC	Nicotinamide	1511010	22251	60	20151203*
Euro OTC	Nicotinamide	1601045	22374	60	20160210*
Euro OTC	Nicotinamide	1610019	22874	40	20161202*
Euro OTC	Nicotinamide	1906027	24799	40	20190712*
Euro OTC	Nicotinamide	2009043	25407	40	20201012*
Euro OTC	Nicotinamide	2203037	26096	40	20220428*
Euro OTC	Nicotinamide	2203037	26096SI	20	20220428*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 480 spectra of 11 reference samples from the substance/substance group *Nicotinamide*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 482 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 640 spectra of 16 reference samples from the substance/substance group *Nicotinamide*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Nicotinamide	11001809	20647	40
Caelo	Nicotinamide	161136	22434	60
Caelo	Nicotinamide	173419	23785	40
Caelo	Nicotinamide	190842	24525	40
Caelo	Nicotinamide	21003053	25861	50
Caelo	Nicotinamide	23002220	26960	40
Euro OTC	Nicotinamide	1707001	23555	40
Euro OTC	Nicotinamide	1801039	23957	40
Euro OTC	Nicotinamide	1812019	24493	40
Euro OTC	Nicotinamide	2001008	25071	40
Euro OTC	Nicotinamide	2105019	25704	50
Euro OTC	Nicotinamide	2309010	26931	40
Fagron	Nicotinamide	23A09-B01-226166	26906	40
Caelo	Nicotinamide	161136	22625	40
Euro OTC	Nicotinamide	2309010	26931SI	20
Fagron	Nicotinamide	23A09-B01-226166	26906SI	20

- 201 444 spectra from a total of 4032 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 147 spectra from 81 *Apo-Ident* customers from 58 batches from the substance/substance group *Nicotinamide*.

- Among them are spectra of independent samples from 55 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Nicotinamide	op12106006	1
AHD	Nicotinamide	2203037-03	1
Caelo	Nicotinamide	12133403	1
Caelo	Nicotinamide	12268302	1
Caelo	Nicotinamide	13097504	1
Caelo	Nicotinamide	13097506	1
Caelo	Nicotinamide	13352002	1
Caelo	Nicotinamide	14246806	1
Caelo	Nicotinamide	1511010-01	1
Caelo	Nicotinamide	1610019-01	1
Caelo	Nicotinamide	16113610	1
Caelo	Nicotinamide	16304803	1
Caelo	Nicotinamide	1707001-01	2
Caelo	Nicotinamide	17104108	2
Caelo	Nicotinamide	17341907	1
Caelo	Nicotinamide	1801039-01	1
Caelo	Nicotinamide	18214803	2
Caelo	Nicotinamide	20004516002	1
Caelo	Nicotinamide	2009043-01	1
Caelo	Nicotinamide	21000112003	2
Caelo	Nicotinamide	21000112006	1
Caelo	Nicotinamide	OP117072026	1
Caesar & Loretz GmbH	Nicotinamide	20004516002	1
DSM Nutritional Prod...	Nicotinamide	1106044-01	1
EuRho/Sanacorp	Nicotinamide	2001008-02	1
EuRho/Sanacorp	Nicotinamide	2009043-01	1
EuRho	Nicotinamide	200100801	1
EuRho	Nicotinamide	2203037-03	1
Euro OTC	Nicotinamide		1
Euro OTC	Nicotinamide	1108021-01	1
Euro OTC	Nicotinamide	11208021	1
Euro OTC	Nicotinamide	11401052	1
Euro OTC	Nicotinamide	1211031-02	5
Euro OTC	Nicotinamide	131002501	1
Euro OTC	Nicotinamide	1310025-01	4
Euro OTC	Nicotinamide	1408019-01	2
Euro OTC	Nicotinamide	1408019-19	1
Euro OTC	Nicotinamide	1503024-02	1
Euro OTC	Nicotinamide	1511010-01	5
Euro OTC	Nicotinamide	160104501	1
Euro OTC	Nicotinamide	1601045-01	5
Euro OTC	Nicotinamide	1610019-01	8
Euro OTC	Nicotinamide	1707001-01	12
Euro OTC	Nicotinamide	1801038-01	1
Euro OTC	Nicotinamide	1801039-01	10
Euro OTC	Nicotinamide	1906027-01	7
Euro OTC	Nicotinamide	1906027-01	1
Euro OTC	Nicotinamide	2001008-01	3
Euro OTC	Nicotinamide	2001008-02	4
Euro OTC	Nicotinamide	200904301	1
Euro OTC	Nicotinamide	2009043-01	7
Euro OTC	Nicotinamide	2009043-02	3
Euro OTC	Nicotinamide	2105019-01	1
Euro OTC	Nicotinamide	2203037-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Nicotinamide	2203037-02	3
Euro OTC	Nicotinamide	2203037-03	1
Euro OTC	Nicotinamide	2610019-01	1
Euro OTC	Nicotinamide	OP11708013	2
Fagron	Nicotinamide	12J02-B03	1
Fagron	Nicotinamide	1801039-01	1
Fagron	Nicotinamide	20D06-F05-369981	1
Fagron	Nicotinamide	20F03-F04-371807	2
Fagron	Nicotinamide	21A14-F02	1
Fagron	Nicotinamide	L14020084	1
Gatt-Koller	Nicotinamide	221406112411	1
Gatt-Koller	Nicotinamide	4456/10104110	1
Gehe	Nicotinamide	2001008-02	1
Noweda	Nicotinamide	12133403	2
Noweda	Nicotinamide	22002418006	1
Phoenix	Nicotinamide	1211031-02	1
Phoenix	Nicotinamide	2001008-01	1
Sanacorp	Nicotinamide	2009043-01	1
Sanacorp	Nicotinamide	22002418003	1
sanacorp	Nicotinamide	oP12106006	1
VDL;16.04.15;5,60EUR	Nicotinamide	1408019-01	1

- 235 920 spectra from 1515 *Apo-Ident* customers from a total of 49 203 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Nicotinamide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Nicotinamide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	480	0	152 482
Type B	0	640	0	201 444
Type C	0	147	0	235 920

The substance/substance group *Nicotinamide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0625 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 95.9184 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21364	22251	7.02	276.46
21643	22251	4.32	276.07
22251	22251	0.00	275.65
22374	22374	0.00	274.28
22874	22874	0.00	273.86
23038	23038	0.00	274.93
23050	23050	0.00	275.03
24799	24799	0.00	276.62
25407	25407	0.00	278.11
26096	26096	0.00	277.58

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Nicotinic acid**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20383-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Nicotinic acid; Acidum nicotinicum

Special notes

When selecting the *Nicotinic acid* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Nicotinic acid	4	3	3

Second-stage model

For differentiation of the substance/substance group *Nicotinic acid* the following second-stage model is used:

- Submodel 12

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Nicotinic acid* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Midazolam hydrochloride	132.41	–
⋮	⋮	⋮
Mesalazine	>50	23.56
Clioquinol	>50	50.27
Miconazole nitrate	>50	60.84
Theophylline-ethylenediamine hydrate	>50	214.38

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Nicotinic acid* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Nicotinic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Nicotinic acid	1906026	24805	40	20190711*
Fagron	Nicotinic acid	14E01-B09-293947	21692	60	AR-15-FG-008938-01
Fagron	Nicotinic acid	16H19-B02-330121	23225	40	AR-17-FG-016013-01
Fagron	Nicotinic acid	21C04-B03-215782	27042	40	20210514

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 180 spectra of 4 reference samples from the substance/substance group *Nicotinic acid*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 152 782 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 5 reference samples from the substance/substance group *Nicotinic acid*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Nicotinic acid	1801021	23954	40
Fagron	Nicotinic acid	18B15-B07-350570	24592	40
Fagron	Nicotinic acid	23A11-B03-229438	26819	40
Fagron	Nicotinic acid	23A11-B03-229438	26819SI	20
Fagron	Nicotinic acid	21C04-B03-215782	27042SI†	20

- 201 924 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 2 *Apo-Ident* customers from 3 batches from the substance/substance group *Nicotinic acid*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
Fagron	Nicotinic acid	L17120080	1
gonmisol	Nicotinic acid	17-18/NCN(P)/B/008	1
Kehr	Nicotinic acid	1801021-01	2

- 236 063 spectra from 1515 *Apo-Ident* customers from a total of 49 256 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Nicotinic acid* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Nicotinic acid* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	180	0	152 782
Type B	0	160	0	201 924
Type C	0	4	0	236 063

The substance/substance group *Nicotinic acid* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21692	21692	0.00	169.44
23225	23225	0.00	166.01
24805	24805	0.00	174.64
27042	23225	7.05	165.84

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Nifedipine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10003587-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Nifedipine; Nifedipinum

Special notes

When selecting the *Nifedipine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Nifedipine	3	1	2

Second-stage model

For differentiation of the substance/substance group *Nifedipine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Nifedipine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Caffeine citrate	168.63	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Nifedipine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Nifedipine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Nifedipine	21B18-F02-378364	26067	40	20210609
Fagron	Nifedipine	22G07-B03-218877	26469	40	230502385
Fagron	Nifedipine	22G07-B03-218877	26469SI	20	230502385
Fagron	Nifedipine	23F29-B05-228724	26900	40	20220803
Fagron	Nifedipine	23F29-B05-228724	26900SI	20	20220803

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 160 spectra of 5 reference samples from the substance/substance group *Nifedipine*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 152 802 spectra from a total of 2839 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 60 spectra of 2 reference samples from the substance/substance group *Nifedipine*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Nifedipine	18K19-B02-363428	25056	40
Fagron	Nifedipine	21B18-F02-378364	26067SI†	20

- 202 024 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 3 *Apo-Ident* customers from 3 batches from the substance/substance group *Nifedipine*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Nifedipine	21829-25-4	1
	Nifedipine	22G07-B03-218877	1
Sanacorp	Nifedipine	22G07-B03	1

- 236 064 spectra from 1515 *Apo-Ident* customers from a total of 49 255 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Nifedipine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Nifedipine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	160	0	152 802
Type B	0	60	0	202 024
Type C	0	3	0	236 064

The substance/substance group *Nifedipine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 90.0000 %)
Type C	100.0000 % (> 99.9011 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26067	26469	32.07	348.10
26469	26469	0.00	350.65
26900	26469	9.86	351.74

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Nitrofurantoin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20698-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Nitrofurantoin; Nitrofurantoinum

Special notes

When selecting the *Nitrofurantoin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Nitrofurantoin	6	3	15

Second-stage model

For differentiation of the substance/substance group *Nitrofurantoin* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Nitrofurantoin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	140.95	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Nitrofurantoin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Nitrofurantoin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Nitrofurantoin	12C30-N03	20698	40	1401461
Fagron	Nitrofurantoin	12C30-N03	20837	40	20120417
Fagron	Nitrofurantoin	13B28-N07	21091	40	20130304
Fagron	Nitrofurantoin	15J15-B06-315225	22257	60	AR-16-FG-003763-01
Fagron	Nitrofurantoin	15J15-B06-315225	22322	60	20151028
Fagron	Nitrofurantoin	21J07-B11-219876	26410	40	230502391
Fagron	Nitrofurantoin	21J07-B11-219876	26410SI	20	230502391
Fagron	Nitrofurantoin	22L02-B01-227369	26550	40	20221227
Fagron	Nitrofurantoin	22L02-B01-227369	26550SI	20	20221227
Fagron	Nitrofurantoin	23E23-B06-232014	26901	40	20230630
Fagron	Nitrofurantoin	23E23-B06-232014	26901SI	20	20230630

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 420 spectra of 11 reference samples from the substance/substance group *Nitrofurantoin*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 542 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Nitrofurantoin*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Nitrofurantoin	11K-21-N23	20836	40
Fagron	Nitrofurantoin	11I07-N11	21273	40
Fagron	Nitrofurantoin	23E23-B07-236326	27189	40

- 201 964 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 28 spectra from 22 *Apo-Ident* customers from 19 batches from the substance/substance group *Nitrofurantoin*.

- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Nitrofurantoin	22L02-B01-227369	1
	Nitrofurantoin	22L02-B01-227369	1
Apotheke am Lindenhof	Nitrofurantoin	15J15-B06	1
Fagron	Nitrofurantoin	11/07-N11	1
Fagron	Nitrofurantoin	11F07-N06	3
Fagron	Nitrofurantoin	12C30-N03	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Nitrofurantoin	12F19-N02	1
Fagron	Nitrofurantoin	13A08-N01	1
Fagron	Nitrofurantoin	13B28-N07	1
Fagron	Nitrofurantoin	13D10-N03	1
Fagron	Nitrofurantoin	15J15-B06	1
Fagron	Nitrofurantoin	15J15-B06-313939	3
Fagron	Nitrofurantoin	15J15-B06-315225	3
Fagron	Nitrofurantoin	15J15-B06-317250	3
Fagron	Nitrofurantoin	15J15-B06-319031	1
Fagron	Nitrofurantoin	201203080296	1
Fagron	Nitrofurantoin	23E23-B07-236326	1
Fagron	Nitrofurantoin	2714I-03527	1
Fagron	Nitrofurantoin	3071403	1
Fagron	Nitrofurantoin	71/14	1

- 236 039 spectra from 1515 *Apo-Ident* customers from a total of 49 239 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Nitrofurantoin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Nitrofurantoin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	120	0	201 964
Type C	0	28	0	236 039

The substance/substance group *Nitrofurantoin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 78.5714 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20698	20698	0.00	257.45
20837	20698	5.69	256.86
21091	22257	37.75	230.80
22257	22257	0.00	248.47
22322	22257	4.50	250.10
26410	26410	0.00	286.32
26550	26410	11.90	285.79
26901	26410	12.99	286.09

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Non-ionic emulsifying alcohol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20467-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Non-ionic emulsifying alcohol; Alcoholes emulsificantes nonionici

Special notes

When selecting the *Non-ionic emulsifying alcohol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Non-ionic emulsifying alcohol	9	3	25

Second-stage model

For differentiation of the substance/substance group *Non-ionic emulsifying alcohol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Non-ionic emulsifying alcohol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Emulsifying cetostearyl alcohol (type A)	22.60	–
Cetomacrogol emulsifying wax 1000 NI	31.30	–
Glycerol monostearate, emulsifying	43.93	–
Cetostearyl alcohol	47.80	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Non-ionic emulsifying alcohol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Non-ionic emulsifying alcohol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
apomix	Non-ionic emulsifying alcohol	NS-8350010216	23274	40	20160718
apomix	Non-ionic emulsifying alcohol	NS-8350010618	24695	40	20180925
apomix	Non-ionic emulsifying alcohol	NS-8350010419	25391	40	20190527
apomix	Non-ionic emulsifying alcohol	NS-8350010720	26585	40	20220722
apomix	Non-ionic emulsifying alcohol	NS-8350010720	26585SI	20	20220722
Bombastus	Non-ionic emulsifying alcohol	19001210	24644	40	20190221
Bombastus	Non-ionic emulsifying alcohol	19001210	24664	40	20190221
Caelo	Non-ionic emulsifying alcohol	13413001	21069	40	1405257
Caelo	Non-ionic emulsifying alcohol	13413001	21524	40	20140116
Caelo	Non-ionic emulsifying alcohol	182021	24282	40	20180725*
Caelo	Non-ionic emulsifying alcohol	20002375001	25511	40	20200731
Caelo	Non-ionic emulsifying alcohol	21001521	25695	50	20210518*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 470 spectra of 12 reference samples from the substance/substance group *Non-ionic emulsifying alcohol*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 492 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 6 reference samples from the substance/substance group *Non-ionic emulsifying alcohol*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Non-ionic emulsifying alcohol	162231	22745	40
Caelo	Non-ionic emulsifying alcohol	171836	23576	40
Caelo	Non-ionic emulsifying alcohol	22003308004	26735	40
apomix	Non-ionic emulsifying alcohol	NS-8350010720	25864	50
apomix	Non-ionic emulsifying alcohol	NS-8350010720	25864SI	10
Caelo	Non-ionic emulsifying alcohol	22003308004	26735SI	20

- 201 884 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 68 spectra from 30 *Apo-Ident* customers from 28 batches from the substance/substance group *Non-ionic emulsifying alcohol*.

- Among them are spectra of independent samples from 25 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Non-ionic emulsifying alcohol	22003308002	1
	Non-ionic emulsifying alcohol	NS-8350010720	1
Bombastus	Non-ionic emulsifying alcohol	18005087P-190119-2	1
Bombastus	Non-ionic emulsifying alcohol	18005087P-190315-2	1
Bombastus	Non-ionic emulsifying alcohol	19001210	2
Bombastus	Non-ionic emulsifying alcohol	267575	2
Bombastus	Non-ionic emulsifying alcohol	274059	1
Bombastus	Non-ionic emulsifying alcohol	278281	4
Bombastus	Non-ionic emulsifying alcohol	284009	2
Bombastus	Non-ionic emulsifying alcohol	292319	8
Bombastus	Non-ionic emulsifying alcohol	295568	6
Bombastus	Non-ionic emulsifying alcohol	2995568	1
Bombastus	Non-ionic emulsifying alcohol	304997	5
Bombastus	Non-ionic emulsifying alcohol	3066	1
Bombastus	Non-ionic emulsifying alcohol	306665	1
Bombastus	Non-ionic emulsifying alcohol	306666	8
Bombastus	Non-ionic emulsifying alcohol	311625	2
Caelo	Non-ionic emulsifying alcohol	12254402	1
Caelo	Non-ionic emulsifying alcohol	14241503	1
Caelo	Non-ionic emulsifying alcohol	15287902	3
Caelo	Non-ionic emulsifying alcohol	18202102	1
Caelo	Non-ionic emulsifying alcohol	19045201	1
Caelo	Non-ionic emulsifying alcohol	20002375001	4
Caelo	Non-ionic emulsifying alcohol	20002375003	2
Caelo	Non-ionic emulsifying alcohol	2002375001	1
Caelo	Non-ionic emulsifying alcohol	21091302	1
Caelo	Non-ionic emulsifying alcohol	311625	1
Caesar & Loretz GmbH	Non-ionic emulsifying alcohol	18202102	1
E Plus	Non-ionic emulsifying alcohol	17043701	1
L11	Non-ionic emulsifying alcohol	17043701	1
L31	Non-ionic emulsifying alcohol	16223104	1
Phönix	Non-ionic emulsifying alcohol	274059	1

- 235 999 spectra from 1515 *Apo-Ident* customers from a total of 49 231 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Non-ionic emulsifying alcohol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Non-ionic emulsifying alcohol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	470	0	152 492
Type B	0	200	0	201 884
Type C	0	68	0	235 999

The substance/substance group *Non-ionic emulsifying alcohol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7234 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 91.1765 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21069	21069	0.00	45.61
21524	25695	10.70	37.52
23274	24282	13.35	46.09
24282	24282	0.00	53.77
24644	24282	12.16	47.47
24664	24282	12.26	51.95
24695	25695	7.41	44.40
25391	21069	17.98	31.30
25511	24282	26.95	59.42
25695	25695	0.00	53.88
26585	25695	17.02	37.66

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Norethisterone acetate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20797-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Norethisterone acetate; Norethisteroni acetas

Special notes

When selecting the *Norethisterone acetate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Norethisterone acetate	7	3	48

Second-stage model

For differentiation of the substance/substance group *Norethisterone acetate* the following second-stage model is used:

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Norethisterone acetate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	118.91	–
⋮	⋮	⋮
Prednicarbate	>50	99.79
Capsaicin	>50	101.88
Oxybutynin hydrochloride	>50	164.96
Alfatradiol	>50	240.32
Sodium citrate	>50	256.65
Tetracaine	>50	262.19
Levocarnitine	>50	268.30
Cyproterone acetate	>50	323.42
Amitriptyline hydrochloride	>50	524.94
Pyridoxal-5-phosphate	>50	548.62
Heparin sodium	>50	633.31
Valine	>50	655.40
Quinine hydrochloride dihydrate	>50	718.33
Methoxsalen	>50	789.25
Ciprofloxacin hydrochloride	>50	1079.05
Amifampridine	>50	2031.34
Sucrose	>50	2266.81
Triclosan	>50	2394.57

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Norethisterone acetate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Norethisterone acetate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Norethisterone acetate	15417004	23122	40	1711489
Caelo	Norethisterone acetate	182252	24395	40	20181031*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Norethisterone acetate	1306033-01	21627	60	1511684
Euro OTC	Norethisterone acetate	2401002	27151	40	20240321*
Euro OTC	Norethisterone acetate	2401002	27151SI	30	20240321*
Fagron	Norethisterone acetate	12L14-N03	20797	40	1401558
Fagron	Norethisterone acetate	17B21-B01-341608	23918	40	20170619
Fagron	Norethisterone acetate	19I30-F02-366139	25364	40	20191127
Fagron	Norethisterone acetate	19I30-F02-366139	25364SI	20	20191127

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 350 spectra of 9 reference samples from the substance/substance group *Norethisterone acetate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 612 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 170 spectra of 5 reference samples from the substance/substance group *Norethisterone acetate*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Norethisterone acetate	2106015	25771	40
Fagron	Norethisterone acetate	14H29-B03-325225	23171	40
Fagron	Norethisterone acetate	23H08-B10-227915	27025	40
Euro OTC	Norethisterone acetate	2106015	25771SI	20
Fagron	Norethisterone acetate	23H08-B10-227915	27025SI	30

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 914 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 63 spectra from 36 *Apo-Ident* customers from 53 batches from the substance/substance group *Norethisterone acetate*.

- Among them are spectra of independent samples from 47 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Bombastus	Norethisterone acetate	13J08-N04	1
Caelo	Norethisterone acetate	15417001	1
Caelo	Norethisterone acetate	15417008	1
Caelo	Norethisterone acetate	16081814	1
Caelo	Norethisterone acetate	17B21-B01-335383	1
Euro OTC	Norethisterone acetate	1306033-02	2
Euro/Phönix	Norethisterone acetate	1306033-01	1
Fagron	Norethisterone acetate		1
Fagron	Norethisterone acetate	12C06-N10	2
Fagron	Norethisterone acetate	13D19-N06	1
Fagron	Norethisterone acetate	13J08-N04	1
Fagron	Norethisterone acetate	14d08-b01-292736	1
Fagron	Norethisterone acetate	14D08-B01-292738	1
Fagron	Norethisterone acetate	14H29-B03	1
Fagron	Norethisterone acetate	14H29-B03-299313	1
Fagron	Norethisterone acetate	14H29-B03-302277	2
Fagron	Norethisterone acetate	14h29-b03-310697	1
Fagron	Norethisterone acetate	14H29-B03-321322	1
Fagron	Norethisterone acetate	14H29-B03-325224	1
Fagron	Norethisterone acetate	17B21-B01	1
Fagron	Norethisterone acetate	17B21-B01-335384	1
Fagron	Norethisterone acetate	17B21-B01-341607	2
Fagron	Norethisterone acetate	17B21-B01-341608	1
Fagron	Norethisterone acetate	17B21-B01-344250	1
Fagron	Norethisterone acetate	18C12-B03-347998	1
Fagron	Norethisterone acetate	18C12-B03-349111	1
Fagron	Norethisterone acetate	18C12-B03-349157	2
Fagron	Norethisterone acetate	18C12-B03-353056	1
Fagron	Norethisterone acetate	18C12-B03-354813	1
Fagron	Norethisterone acetate	18C12-B03-354815	2
Fagron	Norethisterone acetate	18L14-B05	2
Fagron	Norethisterone acetate	18L14-B05-358972	1
Fagron	Norethisterone acetate	18L14-B05-358976	1
Fagron	Norethisterone acetate	18L14-B05-358977	1
Fagron	Norethisterone acetate	19/30-F02-366134	1
Fagron	Norethisterone acetate	19130-F02-373337	1
Fagron	Norethisterone acetate	19I30-F02-366134	1
Fagron	Norethisterone acetate	19I30-f02-366139	1
Fagron	Norethisterone acetate	19I30-F02-366139	1
Fagron	Norethisterone acetate	19I30-F02-3688303	1
Fagron	Norethisterone acetate	21g12-b02-213688	1
Fagron	Norethisterone acetate	21G12-B02-213688	1
Fagron	Norethisterone acetate	21G12-B02-213691	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Norethisterone acetate	21G12-B02	1
Fagron	Norethisterone acetate	22061206	1
Fagron	Norethisterone acetate	23071509	1
Fagron	Norethisterone acetate	F02-3661309	1
Fagron	Norethisterone acetate	F02-3733307	2
Gehe	Norethisterone acetate	14H29-B03-321324	1
Gehe	Norethisterone acetate	15417011	1
GEHE	Norethisterone acetate	18L-14B05	1
Phoenix	Norethisterone acetate	17B21B01335384	1
Phönix	Norethisterone acetate	14H29-B03-315702	1
Phönix	Norethisterone acetate	F02-3661305	1

- 236 004 spectra from 1515 *Apo-Ident* customers from a total of 49 205 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Norethisterone acetate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Norethisterone acetate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	350	0	152 612
Type B	0	170	0	201 914
Type C	0	61	2	236 004

The substance/substance group *Norethisterone acetate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2857 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.4706 %)
Type C	100.0000 % (> 99.9007 %)	96.8254 % (> 92.0635 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20797	20797	0.00	147.33
21627	21627	0.00	141.48
23122	23122	0.00	144.30
23918	24395	3.91	147.63
24395	24395	0.00	147.96
25364	24395	4.52	148.28
27151	27151	0.00	138.05

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Noscapine hydrochloride hydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10006312-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Noscapine hydrochloride hydrate; Noscapini hydrochloridum hydricum

Special notes

When selecting the *Noscapine hydrochloride hydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Noscapine hydrochloride hydrate	3	1	0

Second-stage model

For differentiation of the substance/substance group *Noscapine hydrochloride hydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Noscapine hydrochloride hydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Methacholine chloride	114.82	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Noscapine hydrochloride hydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Noscapine hydrochloride hydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Noscapine hydrochloride h…	23F20-B11-231036	26899	40	240603357
Fagron	Noscapine hydrochloride h…	24C23-B04-235324	27379	40	20240426
Gatt-Koller	Noscapine hydrochloride h…	23J00299	26675	35	240401847

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 115 spectra of 3 reference samples from the substance/substance group *Noscapine hydrochloride hydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.
- 152 847 spectra from a total of 2839 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 100 spectra of 4 reference samples from the substance/substance group *Noscapine hydrochloride hydrate*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Gatt-Koller	Noscapine hydrochloride h…	22J02175	26676	40
Fagron	Noscapine hydrochloride h…	23F20-B11-231036	26899SI†	20
Gatt-Koller	Noscapine hydrochloride h…	23J00299	26675SI†	20
Gatt-Koller	Noscapine hydrochloride h…	22J02175	26676SI	20

- 201 984 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Noscapine hydrochloride hydrate*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Noscapine hydrochloride hydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Noscapine hydrochloride hydrate* and it was evaluated how many matches (positive) and rejections (negative) were

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	115	0	152 847
Type B	0	100	0	201 984
Type C	0	0	0	236 067

The substance/substance group *Noscapine hydrochloride hydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 94.7826 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26675	26675	0.00	205.67
26899	26899	0.00	188.59
27379	26899	77.98	201.39

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Nystatin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20116-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Nystatin; Nystatinum

Special notes

When selecting the *Nystatin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Nystatin	12	7	247

Second-stage model

For differentiation of the substance/substance group *Nystatin* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Nystatin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	54.36	28.25
⋮	⋮	⋮
Bacitracin	>50	15.86
Amphotericin B	>50	21.64
alpha-tocopheryl acetate dry concentrate	>50	33.00
Colistin sulfate	>50	35.81
Cyanocobalamin	>50	36.74
Selenium yeast	>50	41.82
Riboflavin	>50	51.39
Calcium glycerophosphate	>50	56.20
Estradiol hemihydrate	>50	63.12
Estriol	>50	76.76
Triamcinolone	>50	87.61
Calcium pantothenate	>50	93.94
Carmellose sodium	>50	99.72
SyrSpend® SF pH4 neo (Maize starch)	>50	112.33
Gelatine, white	>50	121.88
SyrSpend® SF Alka	>50	133.13
Methylcobalamin	>50	146.52
Hyoscine hydrobromide	>50	151.37
Tosylchloramide sodium	>50	153.08
Rice starch	>50	170.86
Corn starch	>50	213.76
Oxalic acid	>50	240.40
SyrSpend® SF pH4	>50	288.89
Acacia, dried dispersion	>50	320.04
Wheat starch	>50	331.42
Maltodextrin	>50	335.81
Potato starch	>50	354.51
Fructose	>50	518.85

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Nystatin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Nystatin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Nystatin	AP4018717N	23985	40	20160307
Caelo	Nystatin	16272214	23711	40	20160929
Caelo	Nystatin	17025110	23984	40	20170308
Caelo	Nystatin	21004088001	26305	30	20220201
Caelo	Nystatin	21004088001	26305SI	20	20220201
Euro OTC	Nystatin	1712010-01	24103	40	1807445
Euro OTC	Nystatin	1905014	24780	40	20190709*
Euro OTC	Nystatin	2006026	25354	40	20200907*
Euro OTC	Nystatin	2111001	25879	50	20211210*
Euro OTC	Nystatin	2301016	26595	40	20230214*
Euro OTC	Nystatin	2301016	26595SI	20	20230214*
Fagron	Nystatin	19B28-B05-191210	24645	40	20190316
Fagron	Nystatin	19H08-B04-200385	25722	50	20190823
Fagron	Nystatin	22A18-B07-218934	26381	40	20220325
Fagron	Nystatin	22A18-B07-218934	26381SI	20	20220325

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 550 spectra of 15 reference samples from the substance/substance group *Nystatin*. These samples are listed above in the *calibration samples* section. The reference samples come from 12 different batches.
- 152 412 spectra from a total of 2830 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 290 spectra of 8 reference samples from the substance/substance group *Nystatin*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Nystatin	20000969005	25435	40
Caelo	Nystatin	23001392	26843	40
Caelo	Nystatin	24000661	27326	40
Euro OTC	Nystatin	1612001-03	23727	40
Euro OTC	Nystatin	2310010	27005	40
Fagron	Nystatin	16L21-B01-338864	23712	40
Fagron	Nystatin	22I27-B12-225522	26460	40
Euro OTC	Nystatin	2111001	25879SI[†]	10

- 201 794 spectra from a total of 4037 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1880 spectra from 762 *Apo-Ident* customers from 253 batches from the substance/substance group *Nystatin*.
- Among them are spectra of independent samples from 245 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Nystatin		1
	Nystatin	2006026-02	1
	Nystatin	21004088006	1
	Nystatin	211100-02	1
	Nystatin	2111001-03	4
	Nystatin	22002863006	2
	Nystatin	22002863011	6
	Nystatin	230000218004	1
	Nystatin	23000218004	10
	Nystatin	23000218005	2
	Nystatin	23000218006	20
	Nystatin	23001392005	1
	Nystatin	23001392006	1
	Nystatin	2301016-01	33
	Nystatin	2310010-01	9
	Nystatin	24000661004	2
	Nystatin	26001021A	1
	Nystatin	37401222	1
1712010-02	Nystatin	2164071	1
AHC	Nystatin	2301016-01	1
AHD/Euro	Nystatin	1712010-01	1
AHD	Nystatin	1612001-01	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
AHD	Nystatin	18072114	1
AHD	Nystatin	23000218005	1
AHD	Nystatin	23001392004	1
AHD	Nystatin	2301016-01	2
Alliance Healthcare	Nystatin	1905014-03	1
Alliance Healthcare	Nystatin	2006026-01	1
Alliance Healthcare	Nystatin	2006026-02	3
Alliance/EurRho	Nystatin	2006026-0231	1
Alliance	Nystatin	2111001-02	1
Alliance	Nystatin	2301016-01	1
Antibiotice S.A., RO	Nystatin	21000074004	2
Antibiotice SA Iasi/ AHD	Nystatin	1712010-01	1
Antibiotice/Noweda	Nystatin	4019851	3
Antibiotice	Nystatin	1712010-01	2
Anzag	Nystatin	1712010-01	1
Anzag	Nystatin	2310010-01	1
Anzag	Nystatin	2902041-02	1
Apo Ident	Nystatin	2006026-01	1
Apo Ident	Nystatin	800219	1
ApoHo 20.6.17	Nystatin	1722	1
apo-ident/Alliance	Nystatin	2006026-01	1
apo-ident/Phoenix	Nystatin	191220111	1
Apo-ident	Nystatin	1905014-02	1
Apo-ident	Nystatin	2006026-02	2
apomix	Nystatin	2006026-01	1
apomix	Nystatin	2111001-02	1
apotec / AHD	Nystatin	1905014-01	1
apotec	Nystatin	1905014-01	1
Bombastus	Nystatin	1212024-01	1
Caelo	Nystatin	1(18072128)	1
Caelo	Nystatin	11069704	1
Caelo	Nystatin	11069706	2
Caelo	Nystatin	11069716	1
Caelo	Nystatin	11069719	1
Caelo	Nystatin	11069730	1
Caelo	Nystatin	11069731	1
Caelo	Nystatin	1107046-01	1
Caelo	Nystatin	11071894	1
Caelo	Nystatin	12017003	1
Caelo	Nystatin	12017004	4
Caelo	Nystatin	12017009	1
Caelo	Nystatin	12017010	1
Caelo	Nystatin	12017011	2
Caelo	Nystatin	12017015	2
Caelo	Nystatin	12138021	2
Caelo	Nystatin	12158004	3
Caelo	Nystatin	12158005	1
Caelo	Nystatin	12158006	7
Caelo	Nystatin	12158008	3
Caelo	Nystatin	12158009	1
Caelo	Nystatin	12158010	4
Caelo	Nystatin	12158019	3
Caelo	Nystatin	12158020	1
Caelo	Nystatin	12158021	2
Caelo	Nystatin	12158022	1
Caelo	Nystatin	121580921	1
Caelo	Nystatin	12158oo4	1
Caelo	Nystatin	13101201	1
Caelo	Nystatin	13101202	1
Caelo	Nystatin	13173401	8

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Nystatin	13173408	1
Caelo	Nystatin	14363514	1
Caelo	Nystatin	15335310	1
Caelo	Nystatin	1612001	1
Caelo	Nystatin	1612001-03	1
Caelo	Nystatin	16272203	2
Caelo	Nystatin	16L21-B01-338876	1
Caelo	Nystatin	1712010-01	8
Caelo	Nystatin	17400520	1
Caelo	Nystatin	18072014	1
Caelo	Nystatin	18072104	2
Caelo	Nystatin	18072105	6
Caelo	Nystatin	18072107	1
Caelo	Nystatin	18072108	8
Caelo	Nystatin	18072109	11
Caelo	Nystatin	18072112	4
Caelo	Nystatin	18072113	28
Caelo	Nystatin	18072114	18
Caelo	Nystatin	18072118	2
Caelo	Nystatin	18072120	9
Caelo	Nystatin	18072121	8
Caelo	Nystatin	18072123	17
Caelo	Nystatin	18072124	13
Caelo	Nystatin	18072126	2
Caelo	Nystatin	18072128	5
Caelo	Nystatin	18072128P-190709-1	1
Caelo	Nystatin	18072129	4
Caelo	Nystatin	1807213	2
Caelo	Nystatin	183034004	1
Caelo	Nystatin	19026806	1
Caelo	Nystatin	19028801	27
Caelo	Nystatin	19028803	2
Caelo	Nystatin	19028805	1
Caelo	Nystatin	19028806	19
Caelo	Nystatin	19028808	14
Caelo	Nystatin	19028809	27
Caelo	Nystatin	1902881	1
Caelo	Nystatin	19028810	1
Caelo	Nystatin	19028811	1
Caelo	Nystatin	19028813	16
Caelo	Nystatin	1903034005	1
Caelo	Nystatin	19034004	1
Caelo	Nystatin	1905014-01	3
Caelo	Nystatin	1905014-02	1
Caelo	Nystatin	19058809	1
Caelo	Nystatin	19303034009	1
Caelo	Nystatin	193034003	15
Caelo	Nystatin	193034004	21
Caelo	Nystatin	193034005	3
Caelo	Nystatin	193034009	14
Caelo	Nystatin	19304004	1
Caelo	Nystatin	19B28-B06-196732	1
Caelo	Nystatin	20000096006	1
Caelo	Nystatin	2000096006	1
Caelo	Nystatin	20000969002	3
Caelo	Nystatin	20000969005	26
Caelo	Nystatin	20000969006	12
Caelo	Nystatin	2000096902	1
Caelo	Nystatin	20002487001	1
Caelo	Nystatin	20002487004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Nystatin	20004452001	3
Caelo	Nystatin	20004452002	15
Caelo	Nystatin	20004452003	22
Caelo	Nystatin	2000969005	1
Caelo	Nystatin	2006026-02	2
Caelo	Nystatin	2091304	1
Caelo	Nystatin	210000740004	1
Caelo	Nystatin	21000074001	1
Caelo	Nystatin	21000074003	2
Caelo	Nystatin	21000074004	30
Caelo	Nystatin	21000074005	23
Caelo	Nystatin	21000074008	1
Caelo	Nystatin	2100074004	1
Caelo	Nystatin	2100074005	1
Caelo	Nystatin	210021650009	1
Caelo	Nystatin	21002165001	14
Caelo	Nystatin	21002165002	4
Caelo	Nystatin	21002165003	14
Caelo	Nystatin	21002165006	1
Caelo	Nystatin	21002165007	14
Caelo	Nystatin	21002165009	10
Caelo	Nystatin	21004088001	13
Caelo	Nystatin	21004088004	2
Caelo	Nystatin	21004088006	7
Caelo	Nystatin	21004088008	3
Caelo	Nystatin	2111001-03	1
Caelo	Nystatin	22002863002	1
Caelo	Nystatin	22002863006	1
Caelo	Nystatin	22002863010	1
Caelo	Nystatin	22002863011	2
Caelo	Nystatin	23000218006	1
Caelo	Nystatin	3101201	1
Caelo	Nystatin	3338	1
Caelo	Nystatin	4010914	1
Caelo	Nystatin	485870081652	1
Caelo	Nystatin	6082013B	1
Caelo	Nystatin	81072113	1
Caelo	Nystatin	930340031	1
Caelo	Nystatin	C129330	1
Caesar & Loretz GmbH...	Nystatin	18072124	1
Caesar & Loretz GmbH...	Nystatin	1712010-01	1
Caesar & Loretz GmbH...	Nystatin	19028810	1
Caesar & Loretz GmbH...	Nystatin	21004088006	1
Caesar & Loretz GmbH...	Nystatin	18072128	1
Caesar & Loretz GmbH...	Nystatin	19028809	1
Caesar & Loretz GmbH...	Nystatin	19028809	1
Caesar & Loretz GmbH...	Nystatin	21000074005	1
Caesar & Loretz GmbH...	Nystatin	19028813	1
Caesar & Loretz GmbH...	Nystatin	21000074004	1
Caesar & Loretz GmbH...	Nystatin	22002863011	1
Caesar & Loretz GmbH/AEP	Nystatin	23000218004	1
Caesar & Loretz GmbH...	Nystatin	19028809	1
Caesar & Loretz GmbH...	Nystatin	21000074004	1
Caesar & Loretz GmbH...	Nystatin	20004452003	1
Caesar & Loretz GmbH/Gehe	Nystatin	193034004	2
Caesar & Loretz GmbH/Gehe	Nystatin	20000969005	2
Caesar & Loretz GmbH/Gehe	Nystatin	20004452002	1
Caesar & Loretz GmbH...	Nystatin	20004452001	1
Caesar & Loretz GmbH...	Nystatin	19028808	1
Caesar & Loretz GmbH...	Nystatin	21002165001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Nystatin	21002165001	1
Caesar & Loretz GmbH...	Nystatin	193034009	1
Caesar & Loretz GmbH...	Nystatin	21000074004	1
Caesar & Loretz GmbH/K	Nystatin	19028810	1
Caesar & Loretz GmbH/K	Nystatin	21004088001	1
Caesar & Loretz GmbH/kehr	Nystatin	19028813	1
Caesar & Loretz GmbH...	Nystatin	19028813	3
Caesar & Loretz GmbH...	Nystatin	193034009	2
Caesar & Loretz GmbH...	Nystatin	19028808	1
Caesar & Loretz GmbH...	Nystatin	193034009	1
Caesar & Loretz GmbH...	Nystatin	2006026-01	1
Caesar & Loretz GmbH...	Nystatin	21002165003	2
Caesar & Loretz GmbH...	Nystatin	21002165009	1
Caesar & Loretz GmbH...	Nystatin	20000969005	1
Caesar & Loretz GmbH...	Nystatin	21004088001	1
Caesar & Loretz GmbH...	Nystatin	21004088006	1
Caesar & Loretz GmbH...	Nystatin	20000969006	1
Caesar & Loretz GmbH...	Nystatin	210000745005	1
Caesar & Loretz GmbH...	Nystatin	21004088001	1
Caesar & Loretz GmbH/Sa	Nystatin	19028806	1
Caesar & Loretz GmbH...	Nystatin	19028801	1
Caesar & Loretz GmbH...	Nystatin	193034003	1
Caesar & Loretz GmbH...	Nystatin	193034004	1
Caesar & Loretz GmbH...	Nystatin	20000969006	1
Caesar & Loretz GmbH...	Nystatin	20004452002	1
Caesar & Loretz GmbH...	Nystatin	20004452003	1
Caesar & Loretz GmbH...	Nystatin	21000074005	1
Caesar & Loretz GmbH...	Nystatin	21004088008	1
Caesar & Loretz GmbH	Nystatin	18072113	3
Caesar & Loretz GmbH	Nystatin	18072120	1
Caesar & Loretz GmbH	Nystatin	18072123	5
Caesar & Loretz GmbH	Nystatin	18072124	3
Caesar & Loretz GmbH	Nystatin	18072128	3
Caesar & Loretz GmbH	Nystatin	18072129	3
Caesar & Loretz GmbH	Nystatin	19028801	9
Caesar & Loretz GmbH	Nystatin	19028806	3
Caesar & Loretz GmbH	Nystatin	19028808	8
Caesar & Loretz GmbH	Nystatin	19028809	5
Caesar & Loretz GmbH	Nystatin	19028813	5
Caesar & Loretz GmbH	Nystatin	193034003	7
Caesar & Loretz GmbH	Nystatin	193034004	6
Caesar & Loretz GmbH	Nystatin	193034005	4
Caesar & Loretz GmbH	Nystatin	193034009	6
Caesar & Loretz GmbH	Nystatin	20000969002	1
Caesar & Loretz GmbH	Nystatin	20000969005	7
Caesar & Loretz GmbH	Nystatin	20000969006	11
Caesar & Loretz GmbH	Nystatin	20004452001	3
Caesar & Loretz GmbH	Nystatin	20004452002	13
Caesar & Loretz GmbH	Nystatin	20004452003	4
Caesar & Loretz GmbH	Nystatin	2000969006	2
Caesar & Loretz GmbH	Nystatin	21000074003	5
Caesar & Loretz GmbH	Nystatin	21000074004	6
Caesar & Loretz GmbH	Nystatin	21000074005	7
Caesar & Loretz GmbH	Nystatin	21000074008	1
Caesar & Loretz GmbH	Nystatin	21002165001	6
Caesar & Loretz GmbH	Nystatin	21002165002	2
Caesar & Loretz GmbH	Nystatin	21002165007	7
Caesar & Loretz GmbH	Nystatin	21002165009	3
Caesar & Loretz GmbH	Nystatin	21004088001	3
Caesar & Loretz GmbH	Nystatin	21004088004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Nystatin	21004088006	1
Caesar & Loretz GmbH	Nystatin	21004088008	2
Caesar & Loretz GmbH	Nystatin	22002863006	2
Caesar & Loretz GmbH	Nystatin	23000218004	1
Caesar & Loretz Hilden	Nystatin	18072112	2
Caesar & Loretz Hilden	Nystatin	18293404	1
Caesar & Loretz Hilden	Nystatin	19028801	1
Caesar & Loretz/Geil...	Nystatin	19028806	1
Caesar & Loretz/Geil...	Nystatin	19028809	2
Caesar & Loretz/Noweda	Nystatin	193034004	2
Caesar & Loretz/Phoenix	Nystatin	20004452002	1
Caesar&Lorenz / Gehe	Nystatin	19028810	1
Caesar&Lorenz	Nystatin	2100074004	1
Caesar&Lorenz	Nystatin	21002165001	1
Caesar&Lorenz	Nystatin	21002165007	1
Caesar&loretz,AHC	Nystatin	14196509	2
Caesar&loretz,Anzag	Nystatin	12158008	3
Caesar&loretz,Phoenix	Nystatin	1218008	1
Caesar&loretz,Phoenix	Nystatin	13173401	4
Caesar&loretz,Phoenix	Nystatin	13173408	1
Caesar&loretz,Phoenix	Nystatin	14363512	1
caewlo	Nystatin	21004088001	1
Canea Pharma GmbH	Nystatin	18072121	1
Cealo/ AHD	Nystatin	19028801	1
Cealo/Alliance Healthcare	Nystatin	18072118	1
DSM Caïua S.p.A	Nystatin	1207009-01	1
Eu Rho Pharm/ K	Nystatin	2006026-01	1
Eurho Phönix	Nystatin	2006026	1
Eurho Phönix	Nystatin	2111001-02	3
EuRho/Anzag	Nystatin	1107036-01	1
EuRho/Anzag	Nystatin	1712010-02	1
EuRho/Fiebig	Nystatin	1905014-01	4
Eurho/Fiebig	Nystatin	8000219	1
EuRho/Noweda	Nystatin	2006026-02	1
EuRho/Noweda	Nystatin	2111001-02	1
EuRho/Phoenix	Nystatin	1712010-01	2
EuRho/Sanacorp	Nystatin	1712010-02	2
EuRho/Sanacorp	Nystatin	2006026-02	1
Eurho/Synoph	Nystatin	200602-03	4
Eurho/Synoph	Nystatin	2006026-02	1
EuRho	Nystatin	1107046-01	1
EuRho	Nystatin	1207009-01	1
EuRho	Nystatin	1503021-02	2
EuRho	Nystatin	1712010-01	1
EuRho	Nystatin	1905014-02	2
EuRho	Nystatin	2006026-01	1
EuRho	Nystatin	2006026-02	1
EuRho	Nystatin	2111001-02	1
Euro Gehe	Nystatin	1712010-01	1
Euro Noweda	Nystatin	26001021A	1
Euro OTC	Nystatin	1107036-01	4
Euro OTC	Nystatin	1107046-01	2
Euro OTC	Nystatin	1111057-01	7
Euro OTC	Nystatin	1207009-01	7
Euro OTC	Nystatin	1207009-02	2
Euro OTC	Nystatin	121024-01	1
Euro OTC	Nystatin	1212024-01	14
Euro OTC	Nystatin	1212024-02	13
Euro OTC	Nystatin	127009-02	1
Euro OTC	Nystatin	130705301	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Nystatin	1307053-01	5
Euro OTC	Nystatin	1307053-02	2
Euro OTC	Nystatin	1511020-01	1
Euro OTC	Nystatin	1511020-02	1
Euro OTC	Nystatin	16120001-02	1
Euro OTC	Nystatin	1612001-01	4
Euro OTC	Nystatin	1612001-02	1
Euro OTC	Nystatin	161200103	3
Euro OTC	Nystatin	1612001-03	8
Euro OTC	Nystatin	1712010	1
Euro OTC	Nystatin	171201001	1
Euro OTC	Nystatin	1712010-01	99
Euro OTC	Nystatin	171201002	4
Euro OTC	Nystatin	1712010-02	45
Euro OTC	Nystatin	1712010-12	1
Euro OTC	Nystatin	1712020-01	2
Euro OTC	Nystatin	17400520	6
Euro OTC	Nystatin	18072114	1
Euro OTC	Nystatin	18072124	2
Euro OTC	Nystatin	190501-01	1
Euro OTC	Nystatin	19050114-01	1
Euro OTC	Nystatin	1905014	2
Euro OTC	Nystatin	190501401	2
Euro OTC	Nystatin	1905014-01	120
Euro OTC	Nystatin	1905014-02	40
Euro OTC	Nystatin	1905014-03	11
Euro OTC	Nystatin	190514-02	1
Euro OTC	Nystatin	19500711	1
Euro OTC	Nystatin	20006026-01	1
Euro OTC	Nystatin	20006026-02	1
Euro OTC	Nystatin	2003026-01	1
Euro OTC	Nystatin	2006012501	1
Euro OTC	Nystatin	200602302	1
Euro OTC	Nystatin	2006023-02	1
Euro OTC	Nystatin	2006025-2	1
Euro OTC	Nystatin	2006026	1
Euro OTC	Nystatin	2006026-01	47
Euro OTC	Nystatin	200602602	1
Euro OTC	Nystatin	2006026-02	86
Euro OTC	Nystatin	2006026-026	1
Euro OTC	Nystatin	2006026-03	1
Euro OTC	Nystatin	2006026-23	1
Euro OTC	Nystatin	2006226-02	1
Euro OTC	Nystatin	200626-01	2
Euro OTC	Nystatin	200626-02	1
Euro OTC	Nystatin	21000074004	1
Euro OTC	Nystatin	2111001_03	1
Euro OTC	Nystatin	2111001-01	12
Euro OTC	Nystatin	2111001-02	46
Euro OTC	Nystatin	2111001-03	2
Euro OTC	Nystatin	2111011-02	1
Euro OTC	Nystatin	2301016-01	8
Euro OTC	Nystatin	26001021A	1
Euro OTC	Nystatin	2811032-01	1
Euro OTC	Nystatin	4014991	1
Euro OTC	Nystatin	4019851	3
Euro OTC	Nystatin	6026-01	1
Euro OTC	Nystatin	702270	1
Euro OTC	Nystatin	8000219	7
Euro OTC	Nystatin	AP200923-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Nystatin	C129440	1
Euro OTC	Nystatin	C129531	2
Euro OTC	Nystatin	C129854	1
Euro OTC	Nystatin	Nys011222	1
EUro/AHD	Nystatin	1307053-01	1
Euro/Gehe	Nystatin	1905014-01	1
Euro/Gehe	Nystatin	2006026-01	1
Euro/Gehe	Nystatin	2006026-02	1
Euro/Jenne	Nystatin	2006026-02	1
Euro/Phoenix	Nystatin	1905014-03	1
Europharm/Otto	Nystatin	1107046-01	1
Fagron	Nystatin		1
Fagron	Nystatin	11000422a	1
Fagron	Nystatin	11C21-N10	1
Fagron	Nystatin	11K11-No4	1
Fagron	Nystatin	12C29-N09	1
Fagron	Nystatin	12G04-N12	1
Fagron	Nystatin	13C11-N08	1
Fagron	Nystatin	16L21-B01	1
Fagron	Nystatin	17B01-B11-338878	1
Fagron	Nystatin	17J25-B01-344221	1
Fagron	Nystatin	17J25-B01-348043	2
Fagron	Nystatin	18072112	1
Fagron	Nystatin	18900619B	1
Fagron	Nystatin	1905014-01	1
Fagron	Nystatin	19828	1
Fagron	Nystatin	19B28-B05-191208	2
Fagron	Nystatin	19B28-B05-191210	2
Fagron	Nystatin	19H08-B04-200385	2
Fagron	Nystatin	20121202	1
Fagron	Nystatin	20H18-B13-201282	1
Fagron	Nystatin	20H18B13201991	1
Fagron	Nystatin	20H18-B13-201991	2
Fagron	Nystatin	21H13-B01-214453	1
Fagron	Nystatin	4014376	1
Fagron	Nystatin	B01-2144503	1
Fagron	Nystatin	b04-2003805	1
Gatt-Koller	Nystatin	1900206	2
Gehe amax	Nystatin	1712010-01	1
Gehe amax	Nystatin	1905014-01	1
Gehe Rostock	Nystatin	2111001-02	1
Gehe/EuRho	Nystatin	1905014-02	1
Gehe	Nystatin	1107036-01	1
Gehe	Nystatin	1111057-01	1
Gehe	Nystatin	1207009-01	1
Gehe	Nystatin	12158008	1
Gehe	Nystatin	1307053-02	1
Gehe	Nystatin	1712010-01	1
Gehe	Nystatin	1712010-02	1
Gehe	Nystatin	1905014-01	1
Gehe	Nystatin	1905014-03	1
Gehe	Nystatin	20000969005	3
Gehe	Nystatin	200602601	1
Gehe	Nystatin	21000074004	1
GEHE	Nystatin	22002863006	1
Gehe	Nystatin	2301016-01	1
GEHE	Nystatin	2301016-01	1
Geilenkirchen	Nystatin	1905014-01	1
Jenne	Nystatin	21000074003	1
Kehr	Nystatin	1612001-02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Kehr	Nystatin	18072123	1
Kehr	Nystatin	2301016-01	2
L12	Nystatin	1712010-01	1
Nachprüfung	Nystatin	1118E-01941	1
Nachprüfung	Nystatin	123456	1
Noweda Taucha	Nystatin	2111001-01	1
Noweda	Nystatin	1207009-01	1
Noweda	Nystatin	1712010-02	2
Noweda	Nystatin	19028801	1
Noweda	Nystatin	19028808	1
Noweda	Nystatin	21000074005	2
Noweda	Nystatin	21002165001	2
Noweda	Nystatin	2111001-02	1
Noweda	Nystatin	22002863006	2
Noweda	Nystatin	22002863011	1
Noweda	Nystatin	23000218004	2
Noweda	Nystatin	23000218006	1
Noweda	Nystatin	23001392006	1
Noweda	Nystatin	2301016-01	2
Nystatin	Nystatin	1905014-01	1
Otto Geilenkirchen	Nystatin	22002863011	1
Otto Geilenkirchen	Nystatin	2300218004	1
ph.Eur	Nystatin	2111001-02	1
Phoenix/apotec	Nystatin	2301016-01	1
Phoenix	Nystatin	1712010-01	1
Phoenix	Nystatin	1712010-02	1
Phoenix	Nystatin	17400520	1
Phoenix	Nystatin	1905014-01	2
Phoenix	Nystatin	20004452003	1
Phoenix	Nystatin	21002165003	1
Phoenix	Nystatin	23000218005	1
Phoenix	Nystatin	23000218006	1
Phoenix	Nystatin	3361	1
Phoenix	Nystatin	3410	1
Phönix Gotha	Nystatin	1712010-02	1
Phönix/Euro	Nystatin	1111057-01	1
Phönix	Nystatin	12017005	2
Phönix	Nystatin	1212024-01	1
Phönix	Nystatin	1212024-02	1
Phönix	Nystatin	12158010	1
Phönix	Nystatin	1712010-01	1
Phönix	Nystatin	18072109	1
Phönix	Nystatin	18072121	1
Phönix	Nystatin	19028813	1
Phönix	Nystatin	1905014-01	4
Phönix	Nystatin	1905014-02	1
Phönix	Nystatin	1930343004	1
Phönix	Nystatin	20000969005	1
Phönix	Nystatin	2006026-01	1
Phönix	Nystatin	2006026-02	2
Phönix	Nystatin	2111001-01	1
Phönix	Nystatin	23000218006	5
Phönix	Nystatin	2301016-01	1
Phönix	Nystatin	37401222	1
Sanacorp/Caesar & Lo…	Nystatin	18072120	1
Sanacorp/EuRho	Nystatin	171201001	1
Sanacorp	Nystatin	1107046-01	1
Sanacorp	Nystatin	1212024-02	1
sanacorp	Nystatin	19028808	1
Sanacorp	Nystatin	193034009	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Nystatin	20004452002	1
Sanacorp	Nystatin	2002863011	1
Sanacorp	Nystatin	21002165003	1
Sanacorp	Nystatin	21004088006	1
Sanacorp	Nystatin	23000218006	2
Sanacorp	Nystatin	23001392006	1
Sanacorp	Nystatin	2301016-01	4
Sanacorp	Nystatin	24000661003	1
Sanacorp	Nystatin	24000661004	1
VUAB Pharma / Gehe	Nystatin	2006026-02	1
VUAB Pharma	Nystatin	17400520	2
VUAB Pharma	Nystatin	2111001-02	1
VUAB/Noweda	Nystatin	8000219	1

- 234 187 spectra from 1515 *Apo-Ident* customers from a total of 49 012 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Nystatin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Nystatin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	550	0	152 412
Type B	0	290	0	201 794
Type C	0	1760	120	234 187

The substance/substance group *Nystatin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9091 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.9310 %)
Type C	100.0000 % (> 99.9007 %)	93.6170 % (> 93.4574 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested

reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23711	24780	16.83	95.20
23984	26595	19.47	102.63
23985	26595	19.20	105.57
24103	24103	0.00	100.52
24645	24780	16.84	102.75
24780	24780	0.00	103.28
25354	25354	0.00	87.75
25722	24780	26.72	93.13
25879	25879	0.00	79.41
26305	26595	24.87	96.92
26381	24780	8.23	100.45
26595	26595	0.00	106.14

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Octenidine dihydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20759-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Octenidine dihydrochloride; Octenidini dihydrochloridum

Special notes

When selecting the *Octenidine dihydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Octenidine dihydrochloride	10	4	246

Second-stage model

For differentiation of the substance/substance group *Octenidine dihydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Octenidine dihydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	111.46	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Octenidine dihydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Octenidine dihydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Octenidine dihydrochloride	12115202	20759	40	20120511
Caelo	Octenidine dihydrochloride	13071407	20988	40	1407345
Caelo	Octenidine dihydrochloride	13166806	21331	40	20130718
Caelo	Octenidine dihydrochloride	15275502	21888	60	20150910
Caelo	Octenidine dihydrochloride	15356601	21947	60	1604116
Caelo	Octenidine dihydrochloride	15356601	21947SI	60	1604116
Caelo	Octenidine dihydrochloride	170423	23307	40	20170214*
Caelo	Octenidine dihydrochloride	170423	23307SI	40	20170214*
Caelo	Octenidine dihydrochloride	163355	23309	40	20170403*
Caelo	Octenidine dihydrochloride	18223413	24597	40	20181005
Caelo	Octenidine dihydrochloride	18223413	24597SI	40	20181005
Caelo	Octenidine dihydrochloride	23002809	27110	40	20240130*
Caelo	Octenidine dihydrochloride	24002081	27444	40	20240912*
Caelo	Octenidine dihydrochloride	24002081	27444SI	40	20240912*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 620 spectra of 14 reference samples from the substance/substance group *Octenidine dihydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 342 spectra from a total of 2832 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 440 spectra of 10 reference samples from the substance/substance group *Octenidine dihydrochloride*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Octenidine dihydrochloride	160330	22485	60
Caelo	Octenidine dihydrochloride	180174	24023	40
Caelo	Octenidine dihydrochloride	20000606	25202	40
Caelo	Octenidine dihydrochloride	21002272	26010	40
Caelo	Octenidine dihydrochloride	15275502	21888SI†	60
Caelo	Octenidine dihydrochloride	163355	23309SI†	40
Caelo	Octenidine dihydrochloride	180174	24023SI	40
Caelo	Octenidine dihydrochloride	20000606	25202SI	40
Caelo	Octenidine dihydrochloride	21002272	26010SI	40
Caelo	Octenidine dihydrochloride	23002809	27110SI†	40

- 201 644 spectra from a total of 4038 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2656 spectra from 881 *Apo-Ident* customers from 250 batches from the substance/substance group *Octenidine dihydrochloride*.
- Among them are spectra of independent samples from 246 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Octenidine dihydrochloride	21002272002	1
	Octenidine dihydrochloride	21002272011	1
	Octenidine dihydrochloride	21002272012	6
	Octenidine dihydrochloride	21002272018	6
	Octenidine dihydrochloride	21002272020	1
	Octenidine dihydrochloride	21002272022	5
	Octenidine dihydrochloride	21002272024	5
	Octenidine dihydrochloride	21002272025	1
	Octenidine dihydrochloride	2102272024	1
	Octenidine dihydrochloride	22003039002	31
	Octenidine dihydrochloride	220030390021	1
	Octenidine dihydrochloride	22003039003	9
	Octenidine dihydrochloride	22003039004	9
	Octenidine dihydrochloride	22003039005	31
	Octenidine dihydrochloride	22003039008	2
	Octenidine dihydrochloride	22003039009	6
	Octenidine dihydrochloride	2203039002	2
	Octenidine dihydrochloride	23002809002	4
	Octenidine dihydrochloride	23002809003	2
	Octenidine dihydrochloride	23002809004	5
Aep	Octenidine dihydrochloride	22003039004	1
AHC	Octenidine dihydrochloride	20000606005	1
AHD	Octenidine dihydrochloride	16335507	1
AHD	Octenidine dihydrochloride	18197504	1
AHD	Octenidine dihydrochloride	20000606009	1
AHD	Octenidine dihydrochloride	21002272012	2
AHD	Octenidine dihydrochloride	21002272024	2
AHD	Octenidine dihydrochloride	22003039005	5
AHD	Octenidine dihydrochloride	23002809003	1
Alliance Healthcare	Octenidine dihydrochloride	18223403	3
Alliance Healthcare	Octenidine dihydrochloride	18223415	1
Alliance Healthcare	Octenidine dihydrochloride	21002272024	1
Alliance Healthcare	Octenidine dihydrochloride	22003039005	1
Alliance	Octenidine dihydrochloride	22003039002	2
Anzag	Octenidine dihydrochloride	17042602	1
apomix	Octenidine dihydrochloride	13166813	1
Audor Pharma	Octenidine dihydrochloride	17042304	1
Bombastus	Octenidine dihydrochloride	17218506	1
Bombastus	Octenidine dihydrochloride	18017402	1
Cae	Octenidine dihydrochloride	21002272002	1
Caelo	Octenidine dihydrochloride		1
Caelo	Octenidine dihydrochloride	10(20000606019)	1
Caelo	Octenidine dihydrochloride	1000609006	1
Caelo	Octenidine dihydrochloride	11(20004187011)	1
Caelo	Octenidine dihydrochloride	11071925	1
Caelo	Octenidine dihydrochloride	12(20004187011)	1
Caelo	Octenidine dihydrochloride	13061801	1
Caelo	Octenidine dihydrochloride	13166801	1
Caelo	Octenidine dihydrochloride	13166808	2
Caelo	Octenidine dihydrochloride	13166810	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Octenidine dihydrochloride	15006202	3
Caelo	Octenidine dihydrochloride	15006203	1
Caelo	Octenidine dihydrochloride	15006207	5
Caelo	Octenidine dihydrochloride	1515E-03732	1
Caelo	Octenidine dihydrochloride	15275502	8
Caelo	Octenidine dihydrochloride	152755020	1
Caelo	Octenidine dihydrochloride	15275503	3
Caelo	Octenidine dihydrochloride	15275504	1
Caelo	Octenidine dihydrochloride	15356601	6
Caelo	Octenidine dihydrochloride	15356603	4
Caelo	Octenidine dihydrochloride	15356702	1
Caelo	Octenidine dihydrochloride	15356703	9
Caelo	Octenidine dihydrochloride	16032803	8
Caelo	Octenidine dihydrochloride	16032901	2
Caelo	Octenidine dihydrochloride	16032902	4
Caelo	Octenidine dihydrochloride	16032903	2
Caelo	Octenidine dihydrochloride	16032909	7
Caelo	Octenidine dihydrochloride	16032910	6
Caelo	Octenidine dihydrochloride	16033001	2
Caelo	Octenidine dihydrochloride	16033002	2
Caelo	Octenidine dihydrochloride	16277802	9
Caelo	Octenidine dihydrochloride	16302910	1
Caelo	Octenidine dihydrochloride	16325202	1
Caelo	Octenidine dihydrochloride	16325304	11
Caelo	Octenidine dihydrochloride	16325305	14
Caelo	Octenidine dihydrochloride	16325406	6
Caelo	Octenidine dihydrochloride	16325408	2
Caelo	Octenidine dihydrochloride	16325410	3
Caelo	Octenidine dihydrochloride	16335502	3
Caelo	Octenidine dihydrochloride	16335504	23
Caelo	Octenidine dihydrochloride	16335505	4
Caelo	Octenidine dihydrochloride	16335506	1
Caelo	Octenidine dihydrochloride	16335507	11
Caelo	Octenidine dihydrochloride	16335508	8
Caelo	Octenidine dihydrochloride	16335509	20
Caelo	Octenidine dihydrochloride	16335510	12
Caelo	Octenidine dihydrochloride	17042302	8
Caelo	Octenidine dihydrochloride	17042303	6
Caelo	Octenidine dihydrochloride	17042304	13
Caelo	Octenidine dihydrochloride	17042305	5
Caelo	Octenidine dihydrochloride	17042501	1
Caelo	Octenidine dihydrochloride	17042601	1
Caelo	Octenidine dihydrochloride	17042602	9
Caelo	Octenidine dihydrochloride	17042701	1
Caelo	Octenidine dihydrochloride	17042903	21
Caelo	Octenidine dihydrochloride	171116OHC/16335509	1
Caelo	Octenidine dihydrochloride	172118501	1
Caelo	Octenidine dihydrochloride	17218051	1
Caelo	Octenidine dihydrochloride	17218501	45
Caelo	Octenidine dihydrochloride	17218503	15
Caelo	Octenidine dihydrochloride	172185035514	1
Caelo	Octenidine dihydrochloride	17218504	1
Caelo	Octenidine dihydrochloride	17218506	26
Caelo	Octenidine dihydrochloride	17218507	16
Caelo	Octenidine dihydrochloride	17218508	31
Caelo	Octenidine dihydrochloride	17218509	37
Caelo	Octenidine dihydrochloride	17218907	1
Caelo	Octenidine dihydrochloride	1728506	1
Caelo	Octenidine dihydrochloride	1728508	1
Caelo	Octenidine dihydrochloride	18017402	74

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Octenidine dihydrochloride	18017404	1
Caelo	Octenidine dihydrochloride	18197501	52
Caelo	Octenidine dihydrochloride	18197502	23
Caelo	Octenidine dihydrochloride	181975025789	1
Caelo	Octenidine dihydrochloride	18197503	1
Caelo	Octenidine dihydrochloride	18197504	20
Caelo	Octenidine dihydrochloride	181987504	1
Caelo	Octenidine dihydrochloride	18223401	5
Caelo	Octenidine dihydrochloride	18223403	66
Caelo	Octenidine dihydrochloride	18223404	40
Caelo	Octenidine dihydrochloride	18223407	8
Caelo	Octenidine dihydrochloride	18223409	45
Caelo	Octenidine dihydrochloride	18223410	7
Caelo	Octenidine dihydrochloride	18223411	24
Caelo	Octenidine dihydrochloride	18223413	50
Caelo	Octenidine dihydrochloride	18223414	3
Caelo	Octenidine dihydrochloride	18223415	33
Caelo	Octenidine dihydrochloride	18223416	34
Caelo	Octenidine dihydrochloride	18223418	4
Caelo	Octenidine dihydrochloride	18223419	15
Caelo	Octenidine dihydrochloride	18223420	4
Caelo	Octenidine dihydrochloride	18223423	40
Caelo	Octenidine dihydrochloride	18223424	34
Caelo	Octenidine dihydrochloride	18223425	1
Caelo	Octenidine dihydrochloride	18223426	19
Caelo	Octenidine dihydrochloride	18223427	15
Caelo	Octenidine dihydrochloride	18223428	4
Caelo	Octenidine dihydrochloride	1822413	1
Caelo	Octenidine dihydrochloride	18233427	1
Caelo	Octenidine dihydrochloride	1823419	1
Caelo	Octenidine dihydrochloride	190118-03	1
Caelo	Octenidine dihydrochloride	2(18223413)	1
Caelo	Octenidine dihydrochloride	2000006016	1
Caelo	Octenidine dihydrochloride	200000606001	1
Caelo	Octenidine dihydrochloride	200000606005	2
Caelo	Octenidine dihydrochloride	200000606006	2
Caelo	Octenidine dihydrochloride	200000606011	1
Caelo	Octenidine dihydrochloride	200000606012	2
Caelo	Octenidine dihydrochloride	200000606016	2
Caelo	Octenidine dihydrochloride	200004187011	1
Caelo	Octenidine dihydrochloride	2000060002	1
Caelo	Octenidine dihydrochloride	2000060060011	1
Caelo	Octenidine dihydrochloride	200006012	1
Caelo	Octenidine dihydrochloride	20000605007	1
Caelo	Octenidine dihydrochloride	20000606001	31
Caelo	Octenidine dihydrochloride	20000606002	42
Caelo	Octenidine dihydrochloride	20000606005	25
Caelo	Octenidine dihydrochloride	20000606006	55
Caelo	Octenidine dihydrochloride	20000606007	11
Caelo	Octenidine dihydrochloride	20000606008	2
Caelo	Octenidine dihydrochloride	20000606009	17
Caelo	Octenidine dihydrochloride	2000060601	1
Caelo	Octenidine dihydrochloride	20000606010	1
Caelo	Octenidine dihydrochloride	20000606011	28
Caelo	Octenidine dihydrochloride	20000606012	29
Caelo	Octenidine dihydrochloride	20000606015	3
Caelo	Octenidine dihydrochloride	20000606016	23
Caelo	Octenidine dihydrochloride	20000606017	1
Caelo	Octenidine dihydrochloride	20000606018	5
Caelo	Octenidine dihydrochloride	20000606019	44

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Octenidine dihydrochloride	2000060602	1
Caelo	Octenidine dihydrochloride	20000606022	3
Caelo	Octenidine dihydrochloride	2000060606	1
Caelo	Octenidine dihydrochloride	2000060611	1
Caelo	Octenidine dihydrochloride	2000060616	1
Caelo	Octenidine dihydrochloride	2000060619	1
Caelo	Octenidine dihydrochloride	20000620002	7
Caelo	Octenidine dihydrochloride	20004107016	1
Caelo	Octenidine dihydrochloride	2000418012	1
Caelo	Octenidine dihydrochloride	20004187001	29
Caelo	Octenidine dihydrochloride	20004187002	28
Caelo	Octenidine dihydrochloride	20004187003	29
Caelo	Octenidine dihydrochloride	20004187004	4
Caelo	Octenidine dihydrochloride	20004187006	6
Caelo	Octenidine dihydrochloride	20004187009	20
Caelo	Octenidine dihydrochloride	2000418701	1
Caelo	Octenidine dihydrochloride	20004187010	2
Caelo	Octenidine dihydrochloride	20004187011	27
Caelo	Octenidine dihydrochloride	20004187012	31
Caelo	Octenidine dihydrochloride	20004187013	7
Caelo	Octenidine dihydrochloride	20004187014	16
Caelo	Octenidine dihydrochloride	20004187015	23
Caelo	Octenidine dihydrochloride	20004187015(2x)	1
Caelo	Octenidine dihydrochloride	20004187016	15
Caelo	Octenidine dihydrochloride	20004187017	12
Caelo	Octenidine dihydrochloride	2000418704	1
Caelo	Octenidine dihydrochloride	200041871002	1
Caelo	Octenidine dihydrochloride	20004187101	1
Caelo	Octenidine dihydrochloride	200048187006	1
Caelo	Octenidine dihydrochloride	2000606001	1
Caelo	Octenidine dihydrochloride	2000606002	1
Caelo	Octenidine dihydrochloride	2000606006	1
Caelo	Octenidine dihydrochloride	2000606011	1
Caelo	Octenidine dihydrochloride	2000606012	1
Caelo	Octenidine dihydrochloride	2000606019	3
Caelo	Octenidine dihydrochloride	2000606021	1
Caelo	Octenidine dihydrochloride	200060612	1
Caelo	Octenidine dihydrochloride	2000620002	1
Caelo	Octenidine dihydrochloride	2004187002	1
Caelo	Octenidine dihydrochloride	2004187003	2
Caelo	Octenidine dihydrochloride	2004187006	1
Caelo	Octenidine dihydrochloride	2004187009	3
Caelo	Octenidine dihydrochloride	2004187011	1
Caelo	Octenidine dihydrochloride	2100227014	2
Caelo	Octenidine dihydrochloride	21002272001	4
Caelo	Octenidine dihydrochloride	21002272002	23
Caelo	Octenidine dihydrochloride	21002272003	16
Caelo	Octenidine dihydrochloride	21002272004	23
Caelo	Octenidine dihydrochloride	21002272006	12
Caelo	Octenidine dihydrochloride	21002272009	7
Caelo	Octenidine dihydrochloride	21002272011	1
Caelo	Octenidine dihydrochloride	21002272012	7
Caelo	Octenidine dihydrochloride	21002272014	16
Caelo	Octenidine dihydrochloride	21002272015	5
Caelo	Octenidine dihydrochloride	21002272018	13
Caelo	Octenidine dihydrochloride	2100227202	1
Caelo	Octenidine dihydrochloride	21002272020	1
Caelo	Octenidine dihydrochloride	21002272022	11
Caelo	Octenidine dihydrochloride	21002272024	4
Caelo	Octenidine dihydrochloride	21002272025	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Octenidine dihydrochloride	2100272020	1
Caelo	Octenidine dihydrochloride	210906(20004187011)	1
Caelo	Octenidine dihydrochloride	211002272004	1
Caelo	Octenidine dihydrochloride	22003039002	7
Caelo	Octenidine dihydrochloride	22003039005	1
Caelo	Octenidine dihydrochloride	220516(21002272002)	1
Caelo	Octenidine dihydrochloride	220622(21002272002)	1
Caelo	Octenidine dihydrochloride	221222/5	1
Caelo	Octenidine dihydrochloride	2304187009	1
Caelo	Octenidine dihydrochloride	2x2004187002	1
Caelo	Octenidine dihydrochloride	300718A	1
Caelo	Octenidine dihydrochloride	3277	1
Caelo	Octenidine dihydrochloride	3329	1
Caelo	Octenidine dihydrochloride	606007	1
Caelo	Octenidine dihydrochloride	606019	1
Caelo	Octenidine dihydrochloride	6325305	1
Caelo	Octenidine dihydrochloride	718A-03273	1
Caelo	Octenidine dihydrochloride	816M-03732	1
Caelo	Octenidine dihydrochloride	8724	1
Caesar & Lorenz GmbH	Octenidine dihydrochloride	16325410	1
Caesar & Lorenz GmbH	Octenidine dihydrochloride	17218503	1
Caesar & Lorenz GmbH	Octenidine dihydrochloride	18223416	2
Caesar & Lorenz GmbH	Octenidine dihydrochloride	200006006	1
Caesar & Lorenz GmbH	Octenidine dihydrochloride	20000606001	1
Caesar & Lorenz GmbH	Octenidine dihydrochloride	20000606005	1
Caesar & Loretz / Sa…	Octenidine dihydrochloride	18223404	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	16325305	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	18223403	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	20004187009	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	21002272004	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	20004187002	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	21002272014	2
Caesar & Loretz GmbH…	Octenidine dihydrochloride	18223403	2
Caesar & Loretz GmbH…	Octenidine dihydrochloride	18223415	2
Caesar & Loretz GmbH…	Octenidine dihydrochloride	18223428	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	18233415	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	20000606005	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	20000606006	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	20000606012	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	18223416	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	18223426	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	20000606002	1
Caesar & Loretz GmbH/ G	Octenidine dihydrochloride	18223404	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	20004187014	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	20000606002	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	20004187018	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	20004187002	1
Caesar & Loretz GmbH/	Octenidine dihydrochloride	21002272002	1
Caesar & Loretz GmbH/AEP	Octenidine dihydrochloride	20000606009	1
Caesar & Loretz GmbH/AEP	Octenidine dihydrochloride	20004187015	1
Caesar & Loretz GmbH/AHD	Octenidine dihydrochloride	20000606012	1
Caesar & Loretz GmbH/AHD	Octenidine dihydrochloride	21002272003	1
Caesar & Loretz GmbH/AHD	Octenidine dihydrochloride	21002272018	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	20000606011	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	18223423	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	20000606011	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	20000606012	1
Caesar & Loretz GmbH…	Octenidine dihydrochloride	20004187011	1
Caesar & Loretz GmbH/G	Octenidine dihydrochloride	20004187003	1
Caesar & Loretz GmbH/Gehe	Octenidine dihydrochloride	18223413	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Gehe	Octenidine dihydrochloride	20000606006	1
Caesar & Loretz GmbH/Gehe	Octenidine dihydrochloride	20000606009	1
Caesar & Loretz GmbH/Gehe	Octenidine dihydrochloride	20000606010	1
Caesar & Loretz GmbH/Gehe	Octenidine dihydrochloride	20000606012	1
Caesar & Loretz GmbH/GEHE	Octenidine dihydrochloride	20000606012	1
Caesar & Loretz GmbH/GEHE	Octenidine dihydrochloride	20000606018	1
Caesar & Loretz GmbH/Gehe	Octenidine dihydrochloride	20004187003	4
Caesar & Loretz GmbH/Gehe	Octenidine dihydrochloride	20004187009	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20004187012	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20004187002	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	18223411	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20000606002	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20000606005	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20000606016	2
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20004187001	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	21002272011	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	21002272014	2
Caesar & Loretz GmbH/K	Octenidine dihydrochloride	20004187013	1
Caesar & Loretz GmbH/Kehr	Octenidine dihydrochloride	18223418	1
Caesar & Loretz GmbH/Kehr	Octenidine dihydrochloride	21002272025	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	18223425	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20004187015	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	18223423	2
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20000606006	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20000606015	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20000606019	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20004187002	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20004187015	3
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20004187016	3
Caesar & Loretz GmbH...	Octenidine dihydrochloride	21002272022	2
Caesar & Loretz GmbH...	Octenidine dihydrochloride	21002272003	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	21002272004	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	18223416	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	18223423	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20000606019	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20004187003	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20004187006	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	21002272003	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	22003039002	1
Caesar & Loretz GmbH/S	Octenidine dihydrochloride	20004187016	1
Caesar & Loretz GmbH/Sana	Octenidine dihydrochloride	18223415	1
Caesar & Loretz GmbH/Sana	Octenidine dihydrochloride	20000606006	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	18223411	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	18223427	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20004187001	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20004187003	1
Caesar & Loretz GmbH...	Octenidine dihydrochloride	20004187016	1
Caesar & Loretz GmbH	Octenidine dihydrochloride	15006210	1
Caesar & Loretz GmbH	Octenidine dihydrochloride	17218509	2
Caesar & Loretz GmbH	Octenidine dihydrochloride	18017404	1
Caesar & Loretz GmbH	Octenidine dihydrochloride	181975002	1
Caesar & Loretz GmbH	Octenidine dihydrochloride	18197502	2
Caesar & Loretz GmbH	Octenidine dihydrochloride	18223403	3
Caesar & Loretz GmbH	Octenidine dihydrochloride	18223404	3
Caesar & Loretz GmbH	Octenidine dihydrochloride	18223409	1
Caesar & Loretz GmbH	Octenidine dihydrochloride	18223411	4
Caesar & Loretz GmbH	Octenidine dihydrochloride	18223413	7
Caesar & Loretz GmbH	Octenidine dihydrochloride	18223415	2
Caesar & Loretz GmbH	Octenidine dihydrochloride	18223416	2
Caesar & Loretz GmbH	Octenidine dihydrochloride	18223419	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Octenidine dihydrochloride	18223420	3
Caesar & Loretz GmbH	Octenidine dihydrochloride	18223423	5
Caesar & Loretz GmbH	Octenidine dihydrochloride	18223424	7
Caesar & Loretz GmbH	Octenidine dihydrochloride	18223426	5
Caesar & Loretz GmbH	Octenidine dihydrochloride	18223427	4
Caesar & Loretz GmbH	Octenidine dihydrochloride	18223428	2
Caesar & Loretz GmbH	Octenidine dihydrochloride	200006001	1
Caesar & Loretz GmbH	Octenidine dihydrochloride	20000606001	5
Caesar & Loretz GmbH	Octenidine dihydrochloride	20000606002	9
Caesar & Loretz GmbH	Octenidine dihydrochloride	20000606005	9
Caesar & Loretz GmbH	Octenidine dihydrochloride	20000606006	12
Caesar & Loretz GmbH	Octenidine dihydrochloride	20000606007	3
Caesar & Loretz GmbH	Octenidine dihydrochloride	20000606009	5
Caesar & Loretz GmbH	Octenidine dihydrochloride	20000606010	1
Caesar & Loretz GmbH	Octenidine dihydrochloride	20000606011	5
Caesar & Loretz GmbH	Octenidine dihydrochloride	20000606012	7
Caesar & Loretz GmbH	Octenidine dihydrochloride	20000606015	1
Caesar & Loretz GmbH	Octenidine dihydrochloride	20000606016	3
Caesar & Loretz GmbH	Octenidine dihydrochloride	20000606019	18
Caesar & Loretz GmbH	Octenidine dihydrochloride	20000606022	3
Caesar & Loretz GmbH	Octenidine dihydrochloride	200006066005	1
Caesar & Loretz GmbH	Octenidine dihydrochloride	20004187001	9
Caesar & Loretz GmbH	Octenidine dihydrochloride	20004187002	18
Caesar & Loretz GmbH	Octenidine dihydrochloride	20004187003	13
Caesar & Loretz GmbH	Octenidine dihydrochloride	20004187006	4
Caesar & Loretz GmbH	Octenidine dihydrochloride	20004187009	5
Caesar & Loretz GmbH	Octenidine dihydrochloride	20004187010	2
Caesar & Loretz GmbH	Octenidine dihydrochloride	20004187011	10
Caesar & Loretz GmbH	Octenidine dihydrochloride	20004187012	8
Caesar & Loretz GmbH	Octenidine dihydrochloride	20004187013	3
Caesar & Loretz GmbH	Octenidine dihydrochloride	20004187014	7
Caesar & Loretz GmbH	Octenidine dihydrochloride	20004187015	2
Caesar & Loretz GmbH	Octenidine dihydrochloride	20004187016	7
Caesar & Loretz GmbH	Octenidine dihydrochloride	20004187017	8
Caesar & Loretz GmbH	Octenidine dihydrochloride	21002272002	9
Caesar & Loretz GmbH	Octenidine dihydrochloride	21002272003	8
Caesar & Loretz GmbH	Octenidine dihydrochloride	21002272004	9
Caesar & Loretz GmbH	Octenidine dihydrochloride	21002272006	1
Caesar & Loretz GmbH	Octenidine dihydrochloride	21002272009	4
Caesar & Loretz GmbH	Octenidine dihydrochloride	21002272011	3
Caesar & Loretz GmbH	Octenidine dihydrochloride	21002272012	1
Caesar & Loretz GmbH	Octenidine dihydrochloride	21002272014	4
Caesar & Loretz GmbH	Octenidine dihydrochloride	21002272018	5
Caesar & Loretz GmbH	Octenidine dihydrochloride	21002272020	1
Caesar & Loretz GmbH	Octenidine dihydrochloride	21002272022	4
Caesar & Loretz GmbH	Octenidine dihydrochloride	21002272024	4
Caesar & Loretz GmbH	Octenidine dihydrochloride	21002272025	2
Caesar & Loretz GmbH	Octenidine dihydrochloride	22003039002	1
Caesar & Loretz GmbH	Octenidine dihydrochloride	22003039004	2
Caesar & Loretz GmbH	Octenidine dihydrochloride	22003039005	2
Caesar & Loretz Hild…	Octenidine dihydrochloride	20000606005	2
Caesar & Loretz Hild…	Octenidine dihydrochloride	18223403	2
Caesar & Loretz Hild…	Octenidine dihydrochloride	18223413	1
Caesar & Loretz Hild…	Octenidine dihydrochloride	183223424	1
Caesar & Loretz Hild…	Octenidine dihydrochloride	20000606012	1
Caesar & Loretz Hild…	Octenidine dihydrochloride	20000606019	1
Caesar & Loretz Hilden	Octenidine dihydrochloride	18223416	1
Caesar & Loretz Hilden	Octenidine dihydrochloride	20000606006	2
Caesar & Loretz/AHD	Octenidine dihydrochloride	20000606001	1
Caesar & Loretz/Noweda	Octenidine dihydrochloride	20000606019	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz/Noweda	Octenidine dihydrochloride	20004187002	1
Caesar & Loretz	Octenidine dihydrochloride	232215	1
Caesar&Lorenz / Gehe	Octenidine dihydrochloride	18223419	1
Caesar&Lorenz/AHD	Octenidine dihydrochloride	17218508	1
Caesar&Lorenz	Octenidine dihydrochloride	2000487017	1
Caesar&Loretz GmbH, ...	Octenidine dihydrochloride	17042302	1
Caesar&Loretz GmbH	Octenidine dihydrochloride	16335504	1
Caesar&Loretz GmbH	Octenidine dihydrochloride	20000606011	1
Caesar&Loretz GmbH	Octenidine dihydrochloride	21002272011	1
Caleo/ Fiebig	Octenidine dihydrochloride	17218508	2
CALEO/Noweda	Octenidine dihydrochloride	20000606006	1
Caleo	Octenidine dihydrochloride	16033001	1
Caleo	Octenidine dihydrochloride	18197504	1
Caleo	Octenidine dihydrochloride	18223409	1
Caleo	Octenidine dihydrochloride	2000606001	1
Calo, Hilden/ Phönix	Octenidine dihydrochloride	20004187012	1
Calo/Gehe	Octenidine dihydrochloride	16335508	1
Calo/Gehe	Octenidine dihydrochloride	18223404	1
carelo	Octenidine dihydrochloride	22003039005	1
Cealo/Anzag	Octenidine dihydrochloride	211203(20004187015)	1
Cealo/Sanacorp	Octenidine dihydrochloride	15006207	1
Cealo/Sanacorp	Octenidine dihydrochloride	16325305	1
Cealo	Octenidine dihydrochloride	17218507	1
Cealo	Octenidine dihydrochloride	20000606001	1
Cealo5440	Octenidine dihydrochloride	17218501	1
Ceasar & Loretz GmbH...	Octenidine dihydrochloride	16335509	1
Ceasar & Loretz	Octenidine dihydrochloride	20004187012	3
Celo	Octenidine dihydrochloride	16277802	1
Celo	Octenidine dihydrochloride	20000606006	2
Ebert & Jacobi	Octenidine dihydrochloride	16032902	1
Ebert & Jacobi	Octenidine dihydrochloride	16325406	1
EuRho/ AHD	Octenidine dihydrochloride	17218507	1
EuRho/Sanacorp	Octenidine dihydrochloride	16335508	1
Euro OTC	Octenidine dihydrochloride	16032803	1
Euro OTC	Octenidine dihydrochloride	17218501	1
Euro OTC	Octenidine dihydrochloride	18197502	2
Euro OTC	Octenidine dihydrochloride	18223404	1
Euro OTC	Octenidine dihydrochloride	18223413	4
Euro OTC	Octenidine dihydrochloride	20004187014	1
Fagron	Octenidine dihydrochloride	15356601	1
Fagron	Octenidine dihydrochloride	15356703	1
Fagron	Octenidine dihydrochloride	16277802	1
Fagron	Octenidine dihydrochloride	16335507	1
Fagron	Octenidine dihydrochloride	16335510	1
Fagron	Octenidine dihydrochloride	18017402	1
Fagron	Octenidine dihydrochloride	18197501	3
Fagron	Octenidine dihydrochloride	18223403	2
Fagron	Octenidine dihydrochloride	187223403	1
Fagron	Octenidine dihydrochloride	18A12-B03-346964	1
Ferak / Caesar & Lor...	Octenidine dihydrochloride	18197502	1
Ferak Berlin GmbH/ AHD	Octenidine dihydrochloride	20000620002	1
Ferak/Noweda	Octenidine dihydrochloride	202120	1
Ferak/Phoenix	Octenidine dihydrochloride	62120	1
Fiebig	Octenidine dihydrochloride	18017402	1
Fiebig	Octenidine dihydrochloride	20000606009	1
Fresenius	Octenidine dihydrochloride	60715101	1
Gehe 21-01-2019	Octenidine dihydrochloride	18223403	1
Gehe amax	Octenidine dihydrochloride	15356603	1
Gehe amax	Octenidine dihydrochloride	15356703	1
Gehe amax	Octenidine dihydrochloride	16325305	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe amax	Octenidine dihydrochloride	17042305	1
Gehe amax	Octenidine dihydrochloride	17218509	1
Gehe amax	Octenidine dihydrochloride	18197501	1
Gehe amax	Octenidine dihydrochloride	20000606006	1
Gehe Rostock	Octenidine dihydrochloride	18223427	1
Gehe Rostock	Octenidine dihydrochloride	21002272022	1
Gehe	Octenidine dihydrochloride	16032909	2
GEHE	Octenidine dihydrochloride	16325304	1
GEHE	Octenidine dihydrochloride	16325305	1
Gehe	Octenidine dihydrochloride	16335502	1
gehe	Octenidine dihydrochloride	17042602	1
Gehe	Octenidine dihydrochloride	17042903	1
Gehe	Octenidine dihydrochloride	17218501	1
Gehe	Octenidine dihydrochloride	17218508	1
GEHE	Octenidine dihydrochloride	17218509	1
Gehe	Octenidine dihydrochloride	172218508	1
Gehe	Octenidine dihydrochloride	18017402	2
Gehe	Octenidine dihydrochloride	18223401	1
Gehe	Octenidine dihydrochloride	18223403	1
Gehe	Octenidine dihydrochloride	18223419	1
Gehe	Octenidine dihydrochloride	18223424	1
Gehe	Octenidine dihydrochloride	20000606018	1
Gehe	Octenidine dihydrochloride	20004187003	1
gehe	Octenidine dihydrochloride	20004187016	1
Gehe	Octenidine dihydrochloride	20004187016	1
Gehe	Octenidine dihydrochloride	21002272018	1
Gehe	Octenidine dihydrochloride	21002272022	1
Gehe	Octenidine dihydrochloride	21002272024	1
Gehe	Octenidine dihydrochloride	22003039002	2
Gehe	Octenidine dihydrochloride	22003039004	1
Gehe	Octenidine dihydrochloride	22003039005	3
Hepart	Octenidine dihydrochloride	17218508	1
Jenne	Octenidine dihydrochloride	17218507	1
JENNE	Octenidine dihydrochloride	17218508	1
Jenne	Octenidine dihydrochloride	18197502	2
Jenne	Octenidine dihydrochloride	18223416	1
Jenne	Octenidine dihydrochloride	20004187009	1
Kehr	Octenidine dihydrochloride	17218508	1
Kehr	Octenidine dihydrochloride	21002272014	1
Kehr	Octenidine dihydrochloride	21002272018	2
Kehr	Octenidine dihydrochloride	22003039002	2
Kehr	Octenidine dihydrochloride	22003039003	1
Kehr	Octenidine dihydrochloride	22003039004	1
Kehr	Octenidine dihydrochloride	22003039005	1
Kehr	Octenidine dihydrochloride	22003039009	1
Krieger	Octenidine dihydrochloride	20000606019	1
Krieger	Octenidine dihydrochloride	3132	1
Löwen City-Apotheke ...	Octenidine dihydrochloride	2042015	1
Noweda /Cealo	Octenidine dihydrochloride	20000606006	1
Noweda	Octenidine dihydrochloride	16335507	1
Noweda	Octenidine dihydrochloride	17218501	1
Noweda	Octenidine dihydrochloride	18223403	1
Noweda	Octenidine dihydrochloride	18223415	1
Noweda	Octenidine dihydrochloride	18223420	2
Noweda	Octenidine dihydrochloride	1822419	1
Noweda	Octenidine dihydrochloride	20000606019	1
Noweda	Octenidine dihydrochloride	20004187001	1
Noweda	Octenidine dihydrochloride	20004187016	2
Noweda	Octenidine dihydrochloride	20004187017	1
Noweda	Octenidine dihydrochloride	2004187009	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Octenidine dihydrochloride	21002272003no	1
Noweda	Octenidine dihydrochloride	21002272012	1
Noweda	Octenidine dihydrochloride	21002272014	1
Noweda	Octenidine dihydrochloride	21002272024	2
Noweda	Octenidine dihydrochloride	220030309005	1
Noweda	Octenidine dihydrochloride	22003039002	1
Noweda	Octenidine dihydrochloride	22003039005	2
noweda	Octenidine dihydrochloride	22003039008	1
Pheonix	Octenidine dihydrochloride	17218509	1
Phoenix	Octenidine dihydrochloride	17218506	1
Phoenix	Octenidine dihydrochloride	18223415	2
Phoenix	Octenidine dihydrochloride	20000606016	1
Phoenix	Octenidine dihydrochloride	20004187003	2
Phoenix	Octenidine dihydrochloride	20004187016	1
Phoenix	Octenidine dihydrochloride	22003039002	1
Phoenix	Octenidine dihydrochloride	22003039004	1
Phoenix	Octenidine dihydrochloride	22003039005	3
Phoenix	Octenidine dihydrochloride	3033	1
Phoenix	Octenidine dihydrochloride	3040	1
Phoenix	Octenidine dihydrochloride	3107	1
Phoenix	Octenidine dihydrochloride	3113	1
Phoenix	Octenidine dihydrochloride	3221	1
Phoenix	Octenidine dihydrochloride	3419	1
Phoenix	Octenidine dihydrochloride	3423	1
Phönix Gotha	Octenidine dihydrochloride	17218508	1
Phönix	Octenidine dihydrochloride	17218506	1
Phönix	Octenidine dihydrochloride	20000606011	1
Phönix	Octenidine dihydrochloride	20004187003	2
Phönix	Octenidine dihydrochloride	20004187006	1
Phönix	Octenidine dihydrochloride	20004187013	1
Phönix	Octenidine dihydrochloride	2000606019	1
PHÖNIX	Octenidine dihydrochloride	21002272002	1
Phönix	Octenidine dihydrochloride	21002272006	1
Phönix	Octenidine dihydrochloride	21002272018	1
phönix	Octenidine dihydrochloride	22003039005	1
Phönix	Octenidine dihydrochloride	22003039005	7
Phönix	Octenidine dihydrochloride	23002809002	1
Phönix	Octenidine dihydrochloride	23002809004	1
Phönix	Octenidine dihydrochloride	3155	1
sanacorb	Octenidine dihydrochloride	18197502	1
Sanacorp	Octenidine dihydrochloride	16335504	1
Sanacorp	Octenidine dihydrochloride	17218509	1
Sanacorp	Octenidine dihydrochloride	18223426	1
Sanacorp	Octenidine dihydrochloride	22003039002	3
Sanacorp	Octenidine dihydrochloride	22003039005	1
Spangro	Octenidine dihydrochloride	17042305	1

- 233 411 spectra from 1515 *Apo-Ident* customers from a total of 49 012 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Octenidine dihydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Octenidine dihydrochloride*

and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	620	0	152 342
Type B	0	440	0	201 644
Type C	0	2582	74	233 411

The substance/substance group *Octenidine dihydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0323 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6364 %)
Type C	100.0000 % (> 99.9007 %)	97.2139 % (> 97.1009 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20759	27110	8.83	168.21
20988	20988	0.00	164.90
21331	21947	19.73	176.67
21888	21947	3.44	166.01
21947	21947	0.00	168.85
23307	23307	0.00	177.71
23309	23309	0.00	168.59
24597	27110	8.70	168.45
27110	27110	0.00	168.52
27444	27444	0.00	174.87

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ofloxacin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21047-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ofloxacin; Ofloxacinum

Special notes

When selecting the *Ofloxacin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ofloxacin	4	2	12

Second-stage model

For differentiation of the substance/substance group *Ofloxacin* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ofloxacin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Calcium colamine phosphate	78.65	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ofloxacin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ofloxacin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ofloxacin	13A17-N01	21047	40	1403155
Fagron	Ofloxacin	13A17-N01	21052	40	20130123
Fagron	Ofloxacin	13A17-N01	21811	60	20130123
Fagron	Ofloxacin	15H19-B01-312926	21918	60	20151006
Fagron	Ofloxacin	15H19-B01-325226	23090	40	1707611
Fagron	Ofloxacin	18J30-B01-360431	24598	40	20190419

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 6 reference samples from the substance/substance group *Ofloxacin*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 682 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Ofloxacin*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ofloxacin	15H19-B01-337265	23753	40
Fagron	Ofloxacin	22L30-B09-218540	26915	40
Fagron	Ofloxacin	15H19-B01-337265	23754	40
Fagron	Ofloxacin	22L30-B09-218540	26915SI	20

- 201 944 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 17 spectra from 12 *Apo-Ident* customers from 13 batches from the substance/substance group *Ofloxacin*.
- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ofloxacin	22L30-B09-218540	1
Caelo	Ofloxacin	15H19-B01	1
Fagron	Ofloxacin	13A17-N01	2
Fagron	Ofloxacin	15H19-B01-314470	1
Fagron	Ofloxacin	15H19-B01-318532	1
Fagron	Ofloxacin	15H19-B01-337265	1
Fagron	Ofloxacin	15H1-OF-M20150401B	1
Fagron	Ofloxacin	18J30-B01	2
Fagron	Ofloxacin	18J30-B01_363954	1
Fagron	Ofloxacin	18J30-B01-363954	3
Fagron	Ofloxacin	B01-3619609	1
Fagron	Ofloxacin	B01-3639504	1
Fragon	Ofloxacin	15H19-B01-343412	1

- 236 050 spectra from 1515 *Apo-Ident* customers from a total of 49 245 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ofloxacin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ofloxacin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	140	0	201 944
Type C	0	17	0	236 050

The substance/substance group *Ofloxacin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21047	21047	0.00	166.03
21052	21047	6.97	165.19
21811	23090	18.89	146.58
21918	23090	16.18	148.02
23090	23090	0.00	166.84
24598	23090	10.09	171.07

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Omeprazole**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21098-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Omeprazole; Omeprazolum

Special notes

When selecting the *Omeprazole* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Omeprazole	6	3	130

Second-stage model

For differentiation of the substance/substance group *Omeprazole* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Omeprazole* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cyproterone acetate	96.43	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Omeprazole* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Omeprazole*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Omeprazole	15K12-B02-314608	22740	40	20151124
Fagron	Omeprazole	15K12-B02-314608	22890	40	20151124
Fagron	Omeprazole	19F14-B01-362735	24768	40	1910227
Fagron	Omeprazole	20F18-F21-375443	25582	40	20200715
Fagron	Omeprazole	22G08-B01-221106	26384	40	20220714
Fagron	Omeprazole	22L08-B02-225402	26539	40	20221228
Inresa	Omeprazole	OPFP14017	21787	60	1507407
Inresa	Omeprazole	OPFP14017	21796	60	20140228
Inresa	Omeprazole	OPFP14017	22284	60	20140528
Inresa	Omeprazole	OPFP14017	23273	40	20150428

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 460 spectra of 10 reference samples from the substance/substance group *Omeprazole*. These samples are listed above in the *calibration samples* section. The reference samples come from 6

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

different batches.

- 152 502 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 6 reference samples from the substance/substance group *Omeprazole*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Omeprazole	16I20-B03-328940	23272	40
Fagron	Omeprazole	18K01-B03-358185	24583	40
Fagron	Omeprazole	22C31-B01-218818	26151	40
Fagron	Omeprazole	22C31-B01-218818	26151SI	20
Fagron	Omeprazole	22G08-B01-221106	26384SI†	20
Fagron	Omeprazole	22L08-B02-225402	26539SI†	20

- 201 904 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 534 spectra from 192 *Apo-Ident* customers from 145 batches from the substance/substance group *Omeprazole*.

- Among them are spectra of independent samples from 130 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Omeprazole		1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
	Omeprazole	20F18-F21-371963	1
	Omeprazole	21D08-F03-526980	1
	Omeprazole	22C31-B01-218818	3
	Omeprazole	22G08-B01-221106	1
	Omeprazole	22G-08-B01-221106	1
	Omeprazole	22L08-B02-225402	15
	Omeprazole	22L08-B02-225421	1
	Omeprazole	23C16-B08-227714	1
	Omeprazole	23C16-B08-230403	1
	Omeprazole	23C16-B08-230663	1
	Omeprazole	23G31-B06-232416	2
	Omeprazole	23H09-B05-234459	1
	Omeprazole	B06-2324106	1
	Omeprazole	B08-2346505	1
	Omeprazole	OPFP21008	1
	Omeprazole	OPFP21028	2
	Omeprazole	OZ23010	1
AHD	Omeprazole	22L08-B02-225402	4
Alliance Healthcare	Omeprazole	20F18-F21-375443	1
Caelo	Omeprazole	15k12b022314608	1
Caelo	Omeprazole	15K12B02314608	1
Caelo	Omeprazole	16l20-B03-329040	1
Caelo	Omeprazole	17H15-B03	1
Caelo	Omeprazole	17H15-B03-340200	2
Caelo	Omeprazole	17H15-B03342821	1
Caelo	Omeprazole	17K28-B07-348698	6
Caelo	Omeprazole	18E22-B03-353496	1
Caelo	Omeprazole	18K01-B03-358185	1
Caelo	Omeprazole	19F14-B01	1
Caelo	Omeprazole	20f18-f21-371963	1
Caelo	Omeprazole	21D08-F03-526829	1
Caelo	Omeprazole	22444	2
Fagron	Omeprazole		1
Fagron	Omeprazole	15B26-B40-305669	2
Fagron	Omeprazole	15k12-B02	1
Fagron	Omeprazole	15K12-B02	2
Fagron	Omeprazole	15K12-B02-314608	7
Fagron	Omeprazole	15K12-B02-525174	2
Fagron	Omeprazole	16/20-B03	1
Fagron	Omeprazole	16/20-B03-328940	4
Fagron	Omeprazole	16B16-B01-52535	1
Fagron	Omeprazole	16I20-B03-328940	7
Fagron	Omeprazole	16J20-B03-328940	1
Fagron	Omeprazole	16l20-B03-328940	1
Fagron	Omeprazole	17B28-B02	2
Fagron	Omeprazole	17B28-B02-525511	2
Fagron	Omeprazole	17-B28-B02-525511	1
Fagron	Omeprazole	17B28-B02-525557	3
Fagron	Omeprazole	17H15-B03	2
Fagron	Omeprazole	17H15-B03-340200	1
Fagron	Omeprazole	17h15-b03-342821	1
Fagron	Omeprazole	17H15B03342821	1
Fagron	Omeprazole	17H15-B03-342821	18
Fagron	Omeprazole	17h15b0334821	1
Fagron	Omeprazole	17K28-B07	2
Fagron	Omeprazole	17k28b07348698	1
Fagron	Omeprazole	17K28-B07-348698	16
Fagron	Omeprazole	17K28-B07-3486998	1
Fagron	Omeprazole	18E22-B03	1
Fagron	Omeprazole	18e22b03353496	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Omeprazole	18E22B03353496	1
Fagron	Omeprazole	18E22-B03-353496	12
Fagron	Omeprazole	18e22-b03-353496	1
Fagron	Omeprazole	18K01-B03	2
Fagron	Omeprazole	18K01B03358185	2
Fagron	Omeprazole	18K01-B03-358185	16
Fagron	Omeprazole	18K01-B03-358186	2
Fagron	Omeprazole	19F14	1
Fagron	Omeprazole	19F14-B01	4
Fagron	Omeprazole	19F14-B01-362735	14
Fagron	Omeprazole	19f14-B01-363425	1
Fagron	Omeprazole	19F14B01363425	1
Fagron	Omeprazole	19F14-B01-363425	16
Fagron	Omeprazole	19F14-B01-363427	1
Fagron	Omeprazole	19F14-B01-36345	2
Fagron	Omeprazole	19F14-B01-526150	4
Fagron	Omeprazole	19F14B01526150Set19L06-Ko2	1
Fagron	Omeprazole	19F-B01-363425	1
Fagron	Omeprazole	19J29-F03	2
Fagron	Omeprazole	19J29-F03-367825	10
Fagron	Omeprazole	19L09-K02	1
Fagron	Omeprazole	20A16-F02	6
Fagron	Omeprazole	20A16-F02-367834	3
Fagron	Omeprazole	20A16-F02-368827	9
Fagron	Omeprazole	20A16-F02-368828	2
Fagron	Omeprazole	20A16-F02-368827	1
Fagron	Omeprazole	20A416-F02-368827	1
Fagron	Omeprazole	20F18-F21	5
Fagron	Omeprazole	20F18-F21-371963	24
Fagron	Omeprazole	20F18-F21-3754403	1
Fagron	Omeprazole	20F18F21375443	1
Fagron	Omeprazole	20F18-F21-375443	32
Fagron	Omeprazole	20F18-F21-526401	2
Fagron	Omeprazole	20J27-F02	2
Fagron	Omeprazole	20J27-F02-376140	1
Fagron	Omeprazole	20j27-f02-526599	1
Fagron	Omeprazole	20J27-F02-526599	3
Fagron	Omeprazole	20J27F-F02-376140	1
Fagron	Omeprazole	21/01-B05-213885	1
Fagron	Omeprazole	21101-B05-213885	1
Fagron	Omeprazole	21101-BO5-213885	2
Fagron	Omeprazole	21C30-B03	1
Fagron	Omeprazole	21C30-B03-215335	1
Fagron	Omeprazole	21D08F03526829	1
Fagron	Omeprazole	21D08-F03-526829	2
Fagron	Omeprazole	21D08-F03-526980	1
Fagron	Omeprazole	21H04-B12-213937	2
Fagron	Omeprazole	21I01-B05	3
Fagron	Omeprazole	21I01-B05_213885	1
Fagron	Omeprazole	21I01-B05-213885	32
Fagron	Omeprazole	21I01-B05-217276	3
Fagron	Omeprazole	21I1-B05	1
Fagron	Omeprazole	21l01-B05-21028	1
Fagron	Omeprazole	21l01-B05-213885	4
Fagron	Omeprazole	21O01-B05-213885	1
Fagron	Omeprazole	22C31-B01	1
Fagron	Omeprazole	22C31-B01-218672	2
Fagron	Omeprazole	22c31-b01-218818	1
Fagron	Omeprazole	22C31B01218818	1
Fagron	Omeprazole	22C31B-01-218818	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Omeprazole	22C31-B01-218818	21
Fagron	Omeprazole	22C31-B01-21888	1
Fagron	Omeprazole	22C31-B01-218818	2
Fagron	Omeprazole	22G08-B01	1
Fagron	Omeprazole	22G08-B01-221106	16
Fagron	Omeprazole	22L08-B02_225402	1
Fagron	Omeprazole	22L08-B02-225402	8
Fagron	Omeprazole	22L08-B02-2225402	1
Fagron	Omeprazole	20F18-F21-371963	1
Fagron	Omeprazole	20F18-F21-375443	1
Fagron	Omeprazole	70192525	1
Fagron	Omeprazole	73590-58-6	1
Fagron	Omeprazole	b01-2188108	1
Fagron	Omeprazole	B01-3634205	2
Fagron	Omeprazole	B01-526150	2
Fagron	Omeprazole	B05-2138805	3
Fagron	Omeprazole	B05-213885	1
Fagron	Omeprazole	F02-3678304	2
Fagron	Omeprazole	F02-3688207	1
Fagron	Omeprazole	F02-3761400	1
Fagron	Omeprazole	F03-3678205	5
Fagron	Omeprazole	F03-5268209	1
Fagron	Omeprazole	F21-3719603	3
Fagron	Omeprazole	F21-3719605	1
Fagron	Omeprazole	F21-3754403	1
Fagron	Omeprazole	OPFP16030	1
Fagron	Omeprazole	OPFP17033	3
Fagron	Omeprazole	OPFP18052	2
Fagron	Omeprazole	OPFP18052/18K01-B03-358185	1
Fagron	Omeprazole	OPFP19002	3
Fagron	Omeprazole	OPFP19002/19F14-B01-526150	1
Fagron	Omeprazole	OPFP19017	1
Fagron	Omeprazole	OPFP20024	7
Fagron	Omeprazole	OPFP21028	3
Fargon/AHD	Omeprazole	17K28-B07	1
Fargon/AHD	Omeprazole	18K01-B03	1
Fargon/Fiebig	Omeprazole	18K01-B03	1
Fargon/Phönix	Omeprazole	21I01-B05-213885	1
Fargon	Omeprazole	19J29-F03-367825	1
Ferdinand Eimermacher	Omeprazole	4271019	1
Fragon	Omeprazole	17K28-B07-348698	1
Gehe	Omeprazole	17H15-B03-342821	1
Gehe	Omeprazole	19J29-F03-367825	2
Lee Pharma Ltd.	Omeprazole	21101-B05-213885	1
Noveda	Omeprazole	21D08-F03-526980	1
Noweda	Omeprazole	15K15-B02-314608	1
Noweda	Omeprazole	17H15-B03-342821	3
noweda	Omeprazole	19j29-f03-367825	1
Noweda	Omeprazole	22G08-B01-221106	1
Noweda	Omeprazole	22L08-B02-225402	1
Phoenix	Omeprazole	18E22-B03-353496	4
Phönix	Omeprazole	17K28-B07-348698	2
Phönix	Omeprazole	20A16-F02-368827	1
Phönix	Omeprazole	21I01B05213885	1
Phönix	Omeprazole	22C31-B01-218818	4
Sanacorp	Omeprazole	17H15-B03-342821	1
SANACORP	Omeprazole	21I01-B05-213885	1
Sanacorp	Omeprazole	22L08B02225402	1

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 235 533 spectra from 1515 *Apo-Ident* customers from a total of 49 113 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Omeprazole* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Omeprazole* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	460	0	152 502
Type B	0	180	0	201 904
Type C	0	514	20	235 533

The substance/substance group *Omeprazole* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6957 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9007 %)	96.2547 % (> 95.6929 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21787	21787	0.00	96.58
21796	21787	4.75	98.11
22284	21787	4.60	95.45
22740	21787	15.19	93.30
22890	21787	14.90	97.33
23273	21787	6.96	100.77
24768	24768	0.00	121.93
25582	21787	7.65	101.83
26384	21787	5.72	96.08
26539	21787	5.48	96.64

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ornithine aspartate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20842-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ornithine aspartate; Ornithini aspartas

Special notes

When selecting the *Ornithine aspartate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ornithine aspartate	9	4	0

Second-stage model

For differentiation of the substance/substance group *Ornithine aspartate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ornithine aspartate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	80.14	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ornithine aspartate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ornithine aspartate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Ornithine aspartate	1312030-01	21710	60	1506280
Euro OTC	Ornithine aspartate	1611018	22924	40	20161213*
Euro OTC	Ornithine aspartate	1611018-01	23198	40	20161213
Euro OTC	Ornithine aspartate	2301047	26592	40	20230307*
Euro OTC	Ornithine aspartate	2307023	26877	40	20230804*
Euro OTC	Ornithine aspartate	2404004	27404	40	20241104*
Fagron	Ornithine aspartate	14A20-B07-296093	21694	45	1506279
Fagron	Ornithine aspartate	14I24-B04-307758	22599	40	20141110
Fagron	Ornithine aspartate	14I24-B04-307758	22600	40	20141110
Fagron	Ornithine aspartate	17I21-B05-342561	23864	40	1804455

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 425 spectra of 10 reference samples from the substance/substance group *Ornithine aspartate*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 537 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Ornithine aspartate*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ornithine aspartate	1711015	23899	40
Euro OTC	Ornithine aspartate	1805026	24125	40
Euro OTC	Ornithine aspartate	1907037	24859	40
Euro OTC	Ornithine aspartate	2201011	25959	40
Euro OTC	Ornithine aspartate	2201011	25959SI	40
Euro OTC	Ornithine aspartate	2301047	26592SI†	20
Euro OTC	Ornithine aspartate	2307023	26877SI†	20

- 201 844 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Ornithine aspartate*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ornithine aspartate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ornithine aspartate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	425	0	152 537
Type B	0	240	0	201 844
Type C	0	0	0	236 067

The substance/substance group *Ornithine aspartate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5882 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21694	21694	0.00	134.01
21710	21710	0.00	112.60
22599	21694	6.72	134.76
22600	21710	11.74	110.88
22924	22924	0.00	119.50
23198	21694	11.02	138.74
23864	23864	0.00	97.99
26592	26592	0.00	115.12
26877	26877	0.00	114.77
27404	27404	0.00	98.77

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ornithine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20389-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ornithine hydrochloride; Ornithini hydrochloridum

Special notes

When selecting the *Ornithine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ornithine hydrochloride	8	10	15

Second-stage model

For differentiation of the substance/substance group *Ornithine hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ornithine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Glycine	86.39	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ornithine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ornithine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Ornithine hydrochloride	1307028-01	21622	120	20130813
Euro OTC	Ornithine hydrochloride	1605011	22573	40	20160601*
Euro OTC	Ornithine hydrochloride	1612009	22923	40	20170113*
Euro OTC	Ornithine hydrochloride	2001004	25084	40	20200123*
Euro OTC	Ornithine hydrochloride	2004018	25271	40	20200731*
Euro OTC	Ornithine hydrochloride	2305021	26751	40	20230616*
Euro OTC	Ornithine hydrochloride	2305021	26751SI	20	20230616*
Euro OTC	Ornithine hydrochloride	2408003	27391	40	20241029*
Fagron	Ornithine hydrochloride	13A03-N05	20967	40	1403094

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 420 spectra of 9 reference samples from the substance/substance group *Ornithine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 542 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 440 spectra of 12 reference samples from the substance/substance group *Ornithine hydrochloride*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Ornithine hydrochloride	1612009-01	23009	40
Euro OTC	Ornithine hydrochloride	1704006	23159	40
Euro OTC	Ornithine hydrochloride	1803018	24085	40
Euro OTC	Ornithine hydrochloride	1906015	24810	40
Euro OTC	Ornithine hydrochloride	2101021	25547	40
Euro OTC	Ornithine hydrochloride	2103016	25598	40
Euro OTC	Ornithine hydrochloride	2107018	25764	50
Euro OTC	Ornithine hydrochloride	2201012	26042	40
Euro OTC	Ornithine hydrochloride	2301046	26572	40
Euro OTC	Ornithine hydrochloride	2409011	27392	40
Euro OTC	Ornithine hydrochloride	2201012	26042SI	10
Euro OTC	Ornithine hydrochloride	2301046	26572SI	20

- 201 644 spectra from a total of 4035 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 24 spectra from 5 *Apo-Ident* customers from 16 batches from the substance/substance group *Ornithine hydrochloride*.

- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Ornithine hydrochloride	1014I-03475	1
Euro OTC	Ornithine hydrochloride	1704006-01	1
Euro OTC	Ornithine hydrochloride	1906015-01	1
Euro OTC	Ornithine hydrochloride	2001004-01	1
Euro OTC	Ornithine hydrochloride	2004018-01	9
Euro OTC	Ornithine hydrochloride	2101021-01	1
Euro OTC	Ornithine hydrochloride	2103016-01	1
Euro OTC	Ornithine hydrochloride	2107018-01	1
Euro OTC	Ornithine hydrochloride	2201012-01	1
Euro OTC	Ornithine hydrochloride	2201012-02	1
Euro OTC	Ornithine hydrochloride	315E-03475	1
Euro OTC	Ornithine hydrochloride	4712A-03475	1
Euro OTC	Ornithine hydrochloride	516Q-03475	1
Euro OTC	Ornithine hydrochloride	5217M-03475	1
Fagron	Ornithine hydrochloride	13A03-N05	1
Fagron	Ornithine hydrochloride	15A13-B03	1

- 236 043 spectra from 1515 *Apo-Ident* customers from a total of 49 242 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ornithine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ornithine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	440	0	201 644
Type C	0	24	0	236 043

The substance/substance group *Ornithine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6364 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 75.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20967	20967	0.00	201.14
21622	22573	3.25	200.64
22573	22573	0.00	200.75
22923	22923	0.00	200.93
25084	25084	0.00	201.99
25271	25271	0.00	200.24
26751	26751	0.00	201.13
27391	27391	0.00	202.88

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Oxalic acid**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20458-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Oxalic acid; Acidum oxalicum cryst.

Special notes

When selecting the *Oxalic acid* substance/substance group, the following information is displayed to the user:

- Advice: Currently no longer available from major pharmaceutical manufacturers. Therefore, batch maintenance is currently not possible.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Oxalic acid	6	3	27

Second-stage model

For differentiation of the substance/substance group *Oxalic acid* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Oxalic acid* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	84.13	–
⋮	⋮	⋮
Colistin sulfate	>50	55.21
Polymyxin B sulfate	>50	59.25
Riboflavin	>50	70.18
Bacitracin	>50	71.18
Amphotericin B	>50	81.56
Cyanocobalamin	>50	86.50
Tosylchloramide sodium	>50	104.79
Carmellose sodium	>50	108.94
SyrSpend® SF pH4 neo (Maize starch)	>50	112.56
Calcium glycerophosphate	>50	113.60
SyrSpend® SF Alka	>50	126.03
Hyoscine hydrobromide	>50	129.75
Nystatin	>50	135.73
Triamcinolone	>50	137.82
Calcium pantothenate	>50	141.98
Gelatine, white	>50	144.99
Wheat starch	>50	149.53
Estriol	>50	162.26
Rice starch	>50	163.41
Estradiol hemihydrate	>50	169.63
Fructose	>50	172.39
Selenium yeast	>50	185.01
SyrSpend® SF pH4	>50	189.42
Acacia, dried dispersion	>50	193.41
alpha-tocopheryl acetate dry concentrate	>50	226.70
Potato starch	>50	228.37
Corn starch	>50	240.79
Maltodextrin	>50	260.04
Methylcobalamin	>50	291.76

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Oxalic acid* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Oxalic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Oxalic acid	13353901	21042	40	20131029
Caelo	Oxalic acid	12212410	21066	40	1403223
Caelo	Oxalic acid	13353918	21774	60	20131029
Caelo	Oxalic acid	171140	23287	40	20170426*
Caelo	Oxalic acid	171140	23688	40	20170426*
Caelo	Oxalic acid	18202403	24428	40	1905160
Caelo	Oxalic acid	20000475	25207	40	20200313*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 300 spectra of 7 reference samples from the substance/substance group *Oxalic acid*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.
- 152 662 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 4 reference samples from the substance/substance group *Oxalic acid*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Oxalic acid	13353905	21453	60
Caelo	Oxalic acid	20003046	25623	40
Caelo	Oxalic acid	21004224	26007	40

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Oxalic acid	21004224	26007SI	10

- 201 934 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 33 spectra from 27 *Apo-Ident* customers from 29 batches from the substance/substance group *Oxalic acid*.
- Among them are spectra of independent samples from 27 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Oxalic acid	10383104	1
Caelo	Oxalic acid	11111703	1
Caelo	Oxalic acid	12147010	1
Caelo	Oxalic acid	12212406	1
Caelo	Oxalic acid	12212407	1
Caelo	Oxalic acid	12212411	1
Caelo	Oxalic acid	13195413	1
Caelo	Oxalic acid	13195414	1
Caelo	Oxalic acid	13353901	1
Caelo	Oxalic acid	13353905	3
Caelo	Oxalic acid	13353907	2
Caelo	Oxalic acid	13353910	1
Caelo	Oxalic acid	13353915	1
Caelo	Oxalic acid	14334703	1
Caelo	Oxalic acid	15399901	1
Caelo	Oxalic acid	16050205	1
Caelo	Oxalic acid	16297401	1
Caelo	Oxalic acid	17114003	1
Caelo	Oxalic acid	17344503	1
Caelo	Oxalic acid	18196401	1
Caelo	Oxalic acid	4812U-01039	1
Caelo	Oxalic acid	7111808	1
Caelo	Oxalic acid	914E-01039	1
Caelo	Oxalic acid	Retest17111401	2
Caesar & Loretz GmbH...	Oxalic acid	20003046001	1
Caesar & Loretz GmbH	Oxalic acid	20000475004	1
Caesar&Loretz GmbH/ ...	Oxalic acid	13353920	1
Nachprüfung	Oxalic acid		1
sanacorp	Oxalic acid	11098213	1

- 236 034 spectra from 1515 *Apo-Ident* customers from a total of 49 230 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Oxalic acid* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Oxalic acid* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	150	0	201 934
Type C	0	33	0	236 034

The substance/substance group *Oxalic acid* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 81.8182 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21042	21066	6.15	147.35
21066	21066	0.00	141.74
21774	21066	7.08	141.30
23287	23287	0.00	144.73
23688	23688	0.00	144.86
24428	24428	0.00	145.91
25207	25207	0.00	132.15

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Oxetacaine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	23686-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Oxetacaine; Oxetacainum

Special notes

When selecting the *Oxetacaine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Oxetacaine	5	1	20

Second-stage model

For differentiation of the substance/substance group *Oxetacaine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Oxetacaine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Clobetasol propionate	109.99	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Oxetacaine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Oxetacaine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Oxetacaine	APO10-160120	24104	40	1809415
Caelo	Oxetacaine	172498	23686	40	20170925*
Caelo	Oxetacaine	191134	24757	40	20190523*
Euro OTC	Oxetacaine	2002021	25254	40	20200612*
Euro OTC	Oxetacaine	2002020-01	25293	40	20200714

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Oxetacaine*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 762 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 50 spectra of 1 reference samples from the substance/substance group *Oxetacaine*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Oxetacaine	17249805	23916	50

- 202 034 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 87 spectra from 67 *Apo-Ident* customers from 20 batches from the substance/substance group *Oxetacaine*.
- Among them are spectra of independent samples from 20 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Oxetacaine	2002020-03	1
	Oxetacaine	2002020-13	1
	Oxetacaine	21001626004	1
	Oxetacaine	21001626006	5
	Oxetacaine	21001626008	1
Caelo	Oxetacaine	17249805	1
Caelo	Oxetacaine	17249806	1
Caelo	Oxetacaine	17249808	1
Caelo	Oxetacaine	17249809	1
Caelo	Oxetacaine	17249810	6
Caelo	Oxetacaine	191134001	7
Caelo	Oxetacaine	191134002	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Oxetacaine	191134005	5
Caelo	Oxetacaine	191134007	5
Caelo	Oxetacaine	19113401	8
Caelo	Oxetacaine	19113402	9
Caelo	Oxetacaine	21001626002	3
Caelo	Oxetacaine	21001626004	1
Caelo	Oxetacaine	91134002	1
Caesar & Loretz GmbH…	Oxetacaine	191134007	1
Caesar & Loretz GmbH…	Oxetacaine	191134005	1
Caesar & Loretz GmbH…	Oxetacaine	191134007	1
Caesar & Loretz GmbH…	Oxetacaine	19113402	1
Caesar & Loretz GmbH…	Oxetacaine	191134002	2
Caesar & Loretz GmbH	Oxetacaine	191134001	4
CAESAR & LORETZ GMBH	Oxetacaine	191134002	1
Caesar & Loretz GmbH	Oxetacaine	191134005	1
Caesar & Loretz GmbH	Oxetacaine	191134007	2
Caesar&Lorenz	Oxetacaine	191134005	1
EuRho	Oxetacaine	2002021-01	1
Euro OTC	Oxetacaine	2002020-02	1
Euro OTC	Oxetacaine	2002020-03	3
Euro OTC	Oxetacaine	2002021-01	1
Kehr	Oxetacaine	17249805	1

- 235 980 spectra from 1515 *Apo-Ident* customers from a total of 49 238 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Oxetacaine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Oxetacaine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	50	0	202 034
Type C	0	87	0	235 980

The substance/substance group *Oxetacaine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 88.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 93.1034 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23686	23686	0.00	141.70
24104	24104	0.00	147.33
24757	24757	0.00	142.54
25254	25254	0.00	149.69
25293	24104	10.03	145.37

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Oxybuprocaine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20958-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Oxybuprocaine hydrochloride; Oxybuprocaini hydrochloridum

Special notes

When selecting the *Oxybuprocaine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Oxybuprocaine hydrochloride	6	3	17

Second-stage model

For differentiation of the substance/substance group *Oxybuprocaine hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Oxybuprocaine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	111.55	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Oxybuprocaine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Oxybuprocaine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Oxybuprocaine hydrochloride	13D16-N12	20958	40	1402060
Fagron	Oxybuprocaine hydrochloride	13J24-B07-295015	21799	60	AR-15-FG-014812-02
Fagron	Oxybuprocaine hydrochloride	13J24-B07-295015	21799SI	60	AR-15-FG-014812-02
Fagron	Oxybuprocaine hydrochloride	15A26-B07-306787	21922	60	20150203
Fagron	Oxybuprocaine hydrochloride	15A26-B07-306787	21922SI	60	20150203
Fagron	Oxybuprocaine hydrochloride	16L05-B06-334330	23719	40	20170113
Fagron	Oxybuprocaine hydrochloride	16L05-B06-334330	23720	40	20170113
Fagron	Oxybuprocaine hydrochloride	17G21-B03-338576	23745	40	20170823
Fagron	Oxybuprocaine hydrochloride	16L05-B06-334330	23752	40	20170113
Fagron	Oxybuprocaine hydrochloride	19K04-B04-195510	25581	40	20191114

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 480 spectra of 10 reference samples from the substance/substance group *Oxybuprocaine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

samples come from 6 different batches.

- 152 482 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 170 spectra of 4 reference samples from the substance/substance group *Oxybuprocaine hydrochloride*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Oxybuprocaine hydrochloride	18F20-B02-355633	24580	40
Fagron	Oxybuprocaine hydrochloride	20B13-B01-197691	25744	50
Fagron	Oxybuprocaine hydrochloride	20I03-B06-202527	25940	40
Fagron	Oxybuprocaine hydrochloride	20I03-B06-202527	25940SI	40

- 201 914 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 24 spectra from 12 *Apo-Ident* customers from 18 batches from the substance/substance group *Oxybuprocaine hydrochloride*.

- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Oxybuprocaine hydrochloride	14G21B02300384	1
Fagron	Oxybuprocaine hydrochloride	12L19N01	1
Fagron	Oxybuprocaine hydrochloride	13C01-N01	4
Fagron	Oxybuprocaine hydrochloride	13h13-n05	2
Fagron	Oxybuprocaine hydrochloride	13J24B07295015	1
Fagron	Oxybuprocaine hydrochloride	15A26-B07	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Oxybuprocaine hydrochloride	16L05-B06	1
Fagron	Oxybuprocaine hydrochloride	16L05-B06-332495	1
Fagron	Oxybuprocaine hydrochloride	18F20-B02-351233	1
Fagron	Oxybuprocaine hydrochloride	18F20-B02-355633	1
Fagron	Oxybuprocaine hydrochloride	19K04-B04-195510	1
Fagron	Oxybuprocaine hydrochloride	19K04-B04-195511	1
Fagron	Oxybuprocaine hydrochloride	20B13-B01-197691	2
Fagron	Oxybuprocaine hydrochloride	20I03-B06-202527	2
Fagron	Oxybuprocaine hydrochloride	3613N-07321	1
Fagron	Oxybuprocaine hydrochloride	4612M-03639	1
Klenk	Oxybuprocaine hydrochloride	3613M-07321	1
Phönix	Oxybuprocaine hydrochloride	16L05-B06-329642	1

- 236 043 spectra from 1515 *Apo-Ident* customers from a total of 49 240 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Oxybuprocaine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Oxybuprocaine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	480	0	152 482
Type B	0	170	0	201 914
Type C	0	23	1	236 043

The substance/substance group *Oxybuprocaine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.4706 %)
Type C	100.0000 % (> 99.9007 %)	95.8333 % (> 83.3333 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20958	20958	0.00	142.03
21799	21799	0.00	120.27
21922	21799	11.44	136.28
23719	21799	17.80	142.63
23720	21799	15.71	140.47
23745	21799	18.06	142.45
23752	21799	20.96	144.80
25581	21799	16.40	140.11

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Oxybutynin hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20565-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Oxybutynin hydrochloride; Oxybutynini hydrochloridum

Special notes

When selecting the *Oxybutynin hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Oxybutynin hydrochloride	6	8	79

Second-stage model

For differentiation of the substance/substance group *Oxybutynin hydrochloride* the following second-stage model is used:

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Oxybutynin hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prednisolon dihydrogen phosphate di…	116.40	–
⋮	⋮	⋮
Prednicarbate	>50	66.94
Levocarnitine	>50	96.10
Cyproterone acetate	>50	110.21
Capsaicin	>50	110.53
Sodium citrate	>50	145.62
Tetracaine	>50	204.28
Norethisterone acetate	>50	268.17
Alfatradiol	>50	294.99
Amitriptyline hydrochloride	>50	316.58
Quinine hydrochloride dihydrate	>50	326.78
Valine	>50	438.10
Pyridoxal-5-phosphate	>50	440.29
Methoxsalen	>50	468.83
Heparin sodium	>50	548.50
Ciprofloxacin hydrochloride	>50	554.59
Triclosan	>50	1588.05
Amifampridine	>50	1875.42
Sucrose	>50	1955.66

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Oxybutynin hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Oxybutynin hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Oxybutynin hydrochloride	2005030	25351	40	20200911*
Euro OTC	Oxybutynin hydrochloride	2010024	25457	40	20201201*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Oxybutynin hydrochloride	13H26-B03-290572	21543	60	AR-15-FG-002173-01
Fagron	Oxybutynin hydrochloride	14A29-B09-293841	21704	45	20140227
Fagron	Oxybutynin hydrochloride	14I16-B03-312059	22732	40	20141007
Fagron	Oxybutynin hydrochloride	18K22-B01-359482	25059	40	20181217

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 265 spectra of 6 reference samples from the substance/substance group *Oxybutynin hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 697 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 380 spectra of 11 reference samples from the substance/substance group *Oxybutynin hydrochloride*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Oxybutynin hydrochloride	2205010	26189	40
Euro OTC	Oxybutynin hydrochloride	2301024	26578	40
Euro OTC	Oxybutynin hydrochloride	2310011	27062	40
Euro OTC	Oxybutynin hydrochloride	2403009	27211	40
Fagron	Oxybutynin hydrochloride	12D24-N07	20565	40
Fagron	Oxybutynin hydrochloride	16A18-B02-321181	23268	40
Fagron	Oxybutynin hydrochloride	18A12-B03-344347	23995	40
Fagron	Oxybutynin hydrochloride	21H27-B01-220138	26288	40
Euro OTC	Oxybutynin hydrochloride	2205010	26189SI	20
Euro OTC	Oxybutynin hydrochloride	2301024	26578SI	20
Fagron	Oxybutynin hydrochloride	21H27-B01-220138	26288SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 704 spectra from a total of 4037 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 199 spectra from 66 *Apo-Ident* customers from 84 batches from the substance/substance group *Oxybutynin hydrochloride*.

- Among them are spectra of independent samples from 79 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Oxybutynin hydrochloride	21H27-B01-224479	2
	Oxybutynin hydrochloride	21H27-B01-227285	1
	Oxybutynin hydrochloride	B0122013008	1
	Oxybutynin hydrochloride	CC0100362	1
Audor Pharma	Oxybutynin hydrochloride		3
Audor Pharma	Oxybutynin hydrochloride	APOH/043/2017-2018	2
Audor Pharma	Oxybutynin hydrochloride	APOH/067/2018-2019	2
Audor Pharma	Oxybutynin hydrochloride	APOH0122017201810B	2
Audor Pharma	Oxybutynin hydrochloride	APOH0122017-2018-10B	1
Caelo	Oxybutynin hydrochloride	129099	1
Caelo	Oxybutynin hydrochloride	15F05-B03-318524	4
Caelo	Oxybutynin hydrochloride	16/23-B03-328916	1
Caelo	Oxybutynin hydrochloride	16/23-B03-333371	3
Caelo	Oxybutynin hydrochloride	16A18_B02_321181	2
Caelo	Oxybutynin hydrochloride	16A18-B02-321181	3
Caelo	Oxybutynin hydrochloride	16A18-B02-326183	1
Caelo	Oxybutynin hydrochloride	16I23-B03-328916	1
Caelo	Oxybutynin hydrochloride	18A12-B03	2
Caelo	Oxybutynin hydrochloride	18A12-B03-344348	1
Caelo	Oxybutynin hydrochloride	18A12-B03-344350	1
Caelo	Oxybutynin hydrochloride	18A12-Bo3-344350	1
Euro OTC	Oxybutynin hydrochloride	2010024-01	4
Euro OTC	Oxybutynin hydrochloride	2010024-02	1
Fagro/Sanacorp	Oxybutynin hydrochloride	16/23-B03-32891613	1
Fagro/Sanacorp	Oxybutynin hydrochloride	16A18-B02-326183	1
Fagron	Oxybutynin hydrochloride	127979	2
Fagron	Oxybutynin hydrochloride	129099	1
Fagron	Oxybutynin hydrochloride	130563	1
Fagron	Oxybutynin hydrochloride	13H26-B03	1
Fagron	Oxybutynin hydrochloride	13H26-B03-287325	1
Fagron	Oxybutynin hydrochloride	14/16_B03_300207	1
Fagron	Oxybutynin hydrochloride	14/16-B03-300207	5
Fagron	Oxybutynin hydrochloride	14/16-B03-300209	1
Fagron	Oxybutynin hydrochloride	14A29_B09_307322	2
Fagron	Oxybutynin hydrochloride	14a29-b09-307322	2
Fagron	Oxybutynin hydrochloride	14A29-B09-307322	5
Fagron	Oxybutynin hydrochloride	14I16-B03	1
Fagron	Oxybutynin hydrochloride	14I16-B03-300207	1
Fagron	Oxybutynin hydrochloride	15F05_B03_315221	5
Fagron	Oxybutynin hydrochloride	15F05-b03-315220	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Oxybutynin hydrochloride	15F05-B03-315221	6
Fagron	Oxybutynin hydrochloride	15F05-B03-318524	1
Fagron	Oxybutynin hydrochloride	16/23-b03-333371	1
Fagron	Oxybutynin hydrochloride	1607080	1
Fagron	Oxybutynin hydrochloride	16A18-B02-322538	3
Fagron	Oxybutynin hydrochloride	16A18-B02-326183	3
Fagron	Oxybutynin hydrochloride	16I23-B03-328916	3
Fagron	Oxybutynin hydrochloride	16I23-B03-329448	1
Fagron	Oxybutynin hydrochloride	16I23-B03-333371	2
Fagron	Oxybutynin hydrochloride	16l23-b03-328916	1
Fagron	Oxybutynin hydrochloride	170925O/16I23-B03-33	1
Fagron	Oxybutynin hydrochloride	18A12-B03	2
Fagron	Oxybutynin hydrochloride	18A12-B03-344347	1
Fagron	Oxybutynin hydrochloride	18A12-B03-344348	6
Fagron	Oxybutynin hydrochloride	18A12-B03-344350	1
Fagron	Oxybutynin hydrochloride	18A12-B03-345554	1
Fagron	Oxybutynin hydrochloride	18A12-B03-346964	4
Fagron	Oxybutynin hydrochloride	18A12-B03-347807	1
Fagron	Oxybutynin hydrochloride	18A12B03349624	1
Fagron	Oxybutynin hydrochloride	18A12-B03-349624	3
Fagron	Oxybutynin hydrochloride	18A12-B03-350471	3
Fagron	Oxybutynin hydrochloride	18A12-B03-351262	2
Fagron	Oxybutynin hydrochloride	18A12B03352129	1
Fagron	Oxybutynin hydrochloride	18A12-B03-353049	1
Fagron	Oxybutynin hydrochloride	18A23-B03-351262	1
Fagron	Oxybutynin hydrochloride	18K22-B01	2
Fagron	Oxybutynin hydrochloride	18K22-B01-358358	2
Fagron	Oxybutynin hydrochloride	18K22-B01-359482	7
Fagron	Oxybutynin hydrochloride	18K22-B01-363434	1
Fagron	Oxybutynin hydrochloride	18K22-B01-363953	2
Fagron	Oxybutynin hydrochloride	20K100-F04-375776	1
Fagron	Oxybutynin hydrochloride	20K10-F04	1
Fagron	Oxybutynin hydrochloride	20K10-F04	1
Fagron	Oxybutynin hydrochloride	20K10-F04-3757706	2
Fagron	Oxybutynin hydrochloride	20K10-F04-375776	5
Fagron	Oxybutynin hydrochloride	20K10-F04-375777	13
Fagron	Oxybutynin hydrochloride	21G01-F05-379447	9
Fagron	Oxybutynin hydrochloride	21H27-B01-2164002	1
Fagron	Oxybutynin hydrochloride	21H27-B01-218125	3
Fagron	Oxybutynin hydrochloride	21H27-B01-220138	1
Fagron	Oxybutynin hydrochloride	22032E005	1
Fagron	Oxybutynin hydrochloride	22032F004	5
Fagron	Oxybutynin hydrochloride	4375777	1
Fagron	Oxybutynin hydrochloride	5-37944007	1
Fagron	Oxybutynin hydrochloride	F04-3757706	2
Fagron	Oxybutynin hydrochloride	F04-3757707	1
Fagron	Oxybutynin hydrochloride	F04-375776	1
Fagron	Oxybutynin hydrochloride	F05-379449	1
Fagron	Oxybutynin hydrochloride	LCA0100105	1
Fagron	Oxybutynin hydrochloride	OH/044/2020-2021	1
Krieger	Oxybutynin hydrochloride	F04-3757707	1
Noweda	Oxybutynin hydrochloride	18A12-B03-347807	1
Noweda	Oxybutynin hydrochloride	18A12-B03-351262	1
Phoenix	Oxybutynin hydrochloride	16/23-B03-328916	1
Phoenix	Oxybutynin hydrochloride	18A12-B03-346964	1
Phoenix	Oxybutynin hydrochloride	22032E005	2
Phönix	Oxybutynin hydrochloride	18A12-B03-349624	1
Sanacorp	Oxybutynin hydrochloride	18A12-B03-353049	1

- 235 868 spectra from 1515 *Apo-Ident* customers from a total of 49 175 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Oxybutynin hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Oxybutynin hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	265	0	152 697
Type B	0	380	0	201 704
Type C	0	199	0	235 868

The substance/substance group *Oxybutynin hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7358 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.4211 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 96.9849 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21543	21543	0.00	176.31
21704	25457	4.44	174.32
22732	21543	5.03	177.35
25059	25351	9.50	178.42
25351	25351	0.00	179.68
25457	25457	0.00	175.67

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Oxytetracycline hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20090-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Oxytetracycline hydrochloride; Oxytetracyclini hydrochloridum

Special notes

When selecting the *Oxytetracycline hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Oxytetracycline hydrochloride	13	4	150

Second-stage model

For differentiation of the substance/substance group *Oxytetracycline hydrochloride* the following second-stage model is used:

- Submodel 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Oxytetracycline hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	57.63	–
⋮	⋮	⋮
Dequalinium chloride	>50	49.57
Eosin Y	>50	77.50
Tannin	>50	115.48
Levothyroxin sodium	>50	128.08
Dithranol	>50	227.76
Acetylsalicylic acid	>50	393.73
Sodium salicylate	>50	430.92
Benzoic acid	>50	496.47

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Oxytetracycline hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Oxytetracycline hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Oxytetracycline hydrochloride	12130001	20847	40	20120530
Caelo	Oxytetracycline hydrochloride	12328103	21039	40	20121214
Caelo	Oxytetracycline hydrochloride	16077002	22503	40	AR-16-FG-011460-01
Euro OTC	Oxytetracycline hydrochloride	1306022-02	21600	60	1507542
Euro OTC	Oxytetracycline hydrochloride	1506037	21836	60	20150721*
Euro OTC	Oxytetracycline hydrochloride	1506037	21999	60	20150721*
Euro OTC	Oxytetracycline hydrochloride	1602025	22546	40	20160609*
Euro OTC	Oxytetracycline hydrochloride	1602025-01	22658	40	AR-16-FG-014422-01
Euro OTC	Oxytetracycline hydrochloride	1602025	22669	40	20160609*
Euro OTC	Oxytetracycline hydrochloride	1602025-02	22839	40	20161021
Euro OTC	Oxytetracycline hydrochloride	1602025-02	22846	40	20161021
Euro OTC	Oxytetracycline hydrochloride	1701034	23137	40	20170314*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Oxytetracycline hydrochloride	1701035-02	23970	40	20170314
Euro OTC	Oxytetracycline hydrochloride	2103010	25657	40	20210420*
Fagron	Oxytetracycline hydrochloride	13D08-N11	20848	60	20110131
Fagron	Oxytetracycline hydrochloride	15D29-B99-309066	21915	60	20150522

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 740 spectra of 16 reference samples from the substance/substance group *Oxytetracycline - hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 13 different batches.

- 152 222 spectra from a total of 2829 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Oxytetracycline hydrochloride*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Oxytetracycline hydrochloride	173168	23786	40
Euro OTC	Oxytetracycline hydrochloride	1801033	23971	40
Euro OTC	Oxytetracycline hydrochloride	2310021	27275	40
Fagron	Oxytetracycline hydrochloride	15L16-B02-322908	23226	40
Caelo	Oxytetracycline hydrochloride	12130001	20847†	20
Euro OTC	Oxytetracycline hydrochloride	2310021	27275SI	20
Fagron	Oxytetracycline hydrochloride	15L16-B02-322908	23417	40

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 844 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1014 spectra from 431 *Apo-Ident* customers from 167 batches from the substance/substance group *Oxytetracycline hydrochloride*.
- Among them are spectra of independent samples from 149 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Oxytetracycline hydrochloride		1
	Oxytetracycline hydrochloride	10305038	1
	Oxytetracycline hydrochloride	130602202	1
	Oxytetracycline hydrochloride	1306022-02	3
	Oxytetracycline hydrochloride	140701201	1
	Oxytetracycline hydrochloride	2103010-03	5
	Oxytetracycline hydrochloride	2310021-01	2
049	Oxytetracycline hydrochloride	1801033-01	1
AHD	Oxytetracycline hydrochloride	1602025-01	1
AHD	Oxytetracycline hydrochloride	17316805	1
AHD	Oxytetracycline hydrochloride	17316815	1
AHD	Oxytetracycline hydrochloride	1801033-02	1
AHD	Oxytetracycline hydrochloride	2103010-01	1
AHD	Oxytetracycline hydrochloride	21030-10-03	1
Alliance Healthcare	Oxytetracycline hydrochloride	1205028-02	1
Alliance Healthcare	Oxytetracycline hydrochloride	1205222-01	1
Alliance Healthcare	Oxytetracycline hydrochloride	2103010-01	2
Alliance	Oxytetracycline hydrochloride	1407012-03	1
Anzag	Oxytetracycline hydrochloride	12328103	1
Anzag	Oxytetracycline hydrochloride	1506037	1
Anzag	Oxytetracycline hydrochloride	1506037-02	1
Apoident	Oxytetracycline hydrochloride	1602025-01	1
apomix	Oxytetracycline hydrochloride	1602025-02	1
apomix	Oxytetracycline hydrochloride	16077014	1
Bombastus	Oxytetracycline hydrochloride	13L19-B33-290732	1
Bombastus	Oxytetracycline hydrochloride	17316812	1
Bombastus	Oxytetracycline hydrochloride	17316815	1
Bombastus	Oxytetracycline hydrochloride	180103301	1
Caelo	Oxytetracycline hydrochloride	1/01034-02	1
Caelo	Oxytetracycline hydrochloride	11336507	1
Caelo	Oxytetracycline hydrochloride	11336510	3
Caelo	Oxytetracycline hydrochloride	12091405	1
Caelo	Oxytetracycline hydrochloride	12130001	1
Caelo	Oxytetracycline hydrochloride	12328103	1
Caelo	Oxytetracycline hydrochloride	12328104	1
Caelo	Oxytetracycline hydrochloride	12328107	1
Caelo	Oxytetracycline hydrochloride	12G10-N04	1
Caelo	Oxytetracycline hydrochloride	1306022-01	2
Caelo	Oxytetracycline hydrochloride	13L19-B33	1
Caelo	Oxytetracycline hydrochloride	13L19-B33-290730	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Oxytetracycline hydrochloride	1407012-01	1
Caelo	Oxytetracycline hydrochloride	14128003	1
Caelo	Oxytetracycline hydrochloride	14128004	1
Caelo	Oxytetracycline hydrochloride	14I22-B01-301463	1
Caelo	Oxytetracycline hydrochloride	15060108	1
Caelo	Oxytetracycline hydrochloride	15060109	9
Caelo	Oxytetracycline hydrochloride	1506037	1
Caelo	Oxytetracycline hydrochloride	1506037-01	5
Caelo	Oxytetracycline hydrochloride	150603702	1
Caelo	Oxytetracycline hydrochloride	1506037-02	1
Caelo	Oxytetracycline hydrochloride	1602025-01	1
Caelo	Oxytetracycline hydrochloride	160202502	3
Caelo	Oxytetracycline hydrochloride	1602025-02	4
Caelo	Oxytetracycline hydrochloride	16044007	1
Caelo	Oxytetracycline hydrochloride	16077001	3
Caelo	Oxytetracycline hydrochloride	16077002	2
Caelo	Oxytetracycline hydrochloride	16077003	3
Caelo	Oxytetracycline hydrochloride	16077007	2
Caelo	Oxytetracycline hydrochloride	16077008	7
Caelo	Oxytetracycline hydrochloride	16077009	1
Caelo	Oxytetracycline hydrochloride	16077011	2
Caelo	Oxytetracycline hydrochloride	16077012	1
Caelo	Oxytetracycline hydrochloride	16077015	1
Caelo	Oxytetracycline hydrochloride	16077016	2
Caelo	Oxytetracycline hydrochloride	16077017	1
Caelo	Oxytetracycline hydrochloride	1607716	1
Caelo	Oxytetracycline hydrochloride	163406010	1
Caelo	Oxytetracycline hydrochloride	16340605	4
Caelo	Oxytetracycline hydrochloride	16340606	3
Caelo	Oxytetracycline hydrochloride	16340609	1
Caelo	Oxytetracycline hydrochloride	16340610	15
Caelo	Oxytetracycline hydrochloride	16340611	2
Caelo	Oxytetracycline hydrochloride	16340616	1
Caelo	Oxytetracycline hydrochloride	1701034-01	1
Caelo	Oxytetracycline hydrochloride	1701034-02	9
Caelo	Oxytetracycline hydrochloride	1716819	1
Caelo	Oxytetracycline hydrochloride	17316805	6
Caelo	Oxytetracycline hydrochloride	17316806	4
Caelo	Oxytetracycline hydrochloride	17316809	1
Caelo	Oxytetracycline hydrochloride	17316811	4
Caelo	Oxytetracycline hydrochloride	17316812	3
Caelo	Oxytetracycline hydrochloride	17316815	6
Caelo	Oxytetracycline hydrochloride	17316816	1
Caelo	Oxytetracycline hydrochloride	17316819	1
Caelo	Oxytetracycline hydrochloride	17316820	2
Caelo	Oxytetracycline hydrochloride	1801033-01	1
Caelo	Oxytetracycline hydrochloride	21021305	1
Caelo	Oxytetracycline hydrochloride	5041402	1
Caesar & Loretz GmbH...	Oxytetracycline hydrochloride	17316815	2
Caesar & Loretz GmbH	Oxytetracycline hydrochloride	17316815	1
Caesar & Loretz Hilden	Oxytetracycline hydrochloride	17316815	1
Caesar u. Loretz/Noweda	Oxytetracycline hydrochloride	1602025-02	1
Caesar&Loretz GmbH	Oxytetracycline hydrochloride	15060109	1
Caesar&Loretz	Oxytetracycline hydrochloride	16340610	1
caesar	Oxytetracycline hydrochloride	16077008	2
Caleo/ Noweda	Oxytetracycline hydrochloride	16340616	1
Caleo/ Noweda	Oxytetracycline hydrochloride	17316805	1
Century Pharmaceutic...	Oxytetracycline hydrochloride	10305038-0H	1
Century Pharmaceuticals	Oxytetracycline hydrochloride	2103010-01	1
Ebert & Jacobi	Oxytetracycline hydrochloride	1701034-01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Eu Rho Pharm/G	Oxytetracycline hydrochloride	2103010-01	1
EuRho / Gehe	Oxytetracycline hydrochloride	2103010-03	1
EuRho/Alliance Healt…	Oxytetracycline hydrochloride	1801033-01	1
EuRho/Alliance	Oxytetracycline hydrochloride	1801033-01	1
EuRho/Gehe	Oxytetracycline hydrochloride	1801033-02	1
EuRho/Phönix	Oxytetracycline hydrochloride	YT170302019	1
EuRho	Oxytetracycline hydrochloride	1111061-01	1
EuRho	Oxytetracycline hydrochloride	1205028-01	2
EuRho	Oxytetracycline hydrochloride	2103010-03	1
Euro OTC	Oxytetracycline hydrochloride		2
Euro OTC	Oxytetracycline hydrochloride	1011045-01	3
Euro OTC	Oxytetracycline hydrochloride	10305038	1
Euro OTC	Oxytetracycline hydrochloride	10305038-OH	3
Euro OTC	Oxytetracycline hydrochloride	1111061-01	6
Euro OTC	Oxytetracycline hydrochloride	1111061-61	1
Euro OTC	Oxytetracycline hydrochloride	11701034-02	1
Euro OTC	Oxytetracycline hydrochloride	1205028	1
Euro OTC	Oxytetracycline hydrochloride	12050-28	1
Euro OTC	Oxytetracycline hydrochloride	1205028-01	6
Euro OTC	Oxytetracycline hydrochloride	120502802	2
Euro OTC	Oxytetracycline hydrochloride	1205028-02	14
Euro OTC	Oxytetracycline hydrochloride	1306022	1
Euro OTC	Oxytetracycline hydrochloride	130602201	2
Euro OTC	Oxytetracycline hydrochloride	1306022-01	24
Euro OTC	Oxytetracycline hydrochloride	130602202	1
Euro OTC	Oxytetracycline hydrochloride	1306022-02	14
Euro OTC	Oxytetracycline hydrochloride	1306022-03	5
Euro OTC	Oxytetracycline hydrochloride	1407011202	1
Euro OTC	Oxytetracycline hydrochloride	1407012-01	17
Euro OTC	Oxytetracycline hydrochloride	1407012-02	17
Euro OTC	Oxytetracycline hydrochloride	140701203	1
Euro OTC	Oxytetracycline hydrochloride	1407012-03	5
Euro OTC	Oxytetracycline hydrochloride	1407012-09	1
Euro OTC	Oxytetracycline hydrochloride	1407012-1	1
Euro OTC	Oxytetracycline hydrochloride	15051507	1
Euro OTC	Oxytetracycline hydrochloride	15060109	1
Euro OTC	Oxytetracycline hydrochloride	1506037	3
Euro OTC	Oxytetracycline hydrochloride	150603701	1
Euro OTC	Oxytetracycline hydrochloride	1506037-01	31
Euro OTC	Oxytetracycline hydrochloride	1506037-02	32
Euro OTC	Oxytetracycline hydrochloride	1506037-03	19
Euro OTC	Oxytetracycline hydrochloride	15060377-01	1
Euro OTC	Oxytetracycline hydrochloride	16020228-02	1
Euro OTC	Oxytetracycline hydrochloride	1602025	3
Euro OTC	Oxytetracycline hydrochloride	1602025_01	1
Euro OTC	Oxytetracycline hydrochloride	160202501	2
Euro OTC	Oxytetracycline hydrochloride	1602025-01	23
Euro OTC	Oxytetracycline hydrochloride	160202502	1
Euro OTC	Oxytetracycline hydrochloride	1602025-02	55
Euro OTC	Oxytetracycline hydrochloride	1602025-1	1
Euro OTC	Oxytetracycline hydrochloride	162025-02	1
Euro OTC	Oxytetracycline hydrochloride	170034-01	1
Euro OTC	Oxytetracycline hydrochloride	17010301	1
Euro OTC	Oxytetracycline hydrochloride	1701034	1
Euro OTC	Oxytetracycline hydrochloride	170103401	2
Euro OTC	Oxytetracycline hydrochloride	1701034-01	51
Euro OTC	Oxytetracycline hydrochloride	1701034-0104915216	1
Euro OTC	Oxytetracycline hydrochloride	1701034-015415	1
Euro OTC	Oxytetracycline hydrochloride	170103402	3
Euro OTC	Oxytetracycline hydrochloride	1701034-02	59

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Oxytetracycline hydrochloride	170313OH/1602025-01	1
Euro OTC	Oxytetracycline hydrochloride	170612181	1
Euro OTC	Oxytetracycline hydrochloride	171034-02	1
Euro OTC	Oxytetracycline hydrochloride	18010322-02	1
Euro OTC	Oxytetracycline hydrochloride	1801033	6
Euro OTC	Oxytetracycline hydrochloride	1801033_02	1
Euro OTC	Oxytetracycline hydrochloride	180103301	5
Euro OTC	Oxytetracycline hydrochloride	1801033-01	92
Euro OTC	Oxytetracycline hydrochloride	1801033-01P-190311-2	1
Euro OTC	Oxytetracycline hydrochloride	180103302	3
Euro OTC	Oxytetracycline hydrochloride	1801033-02	56
Euro OTC	Oxytetracycline hydrochloride	1801033-1	1
Euro OTC	Oxytetracycline hydrochloride	1801033-22	1
Euro OTC	Oxytetracycline hydrochloride	181016183	1
Euro OTC	Oxytetracycline hydrochloride	2102010-03	1
Euro OTC	Oxytetracycline hydrochloride	210301001	1
Euro OTC	Oxytetracycline hydrochloride	2103010-01	49
Euro OTC	Oxytetracycline hydrochloride	210301002	1
Euro OTC	Oxytetracycline hydrochloride	2103010-02	11
Euro OTC	Oxytetracycline hydrochloride	2103010-03	21
Euro OTC	Oxytetracycline hydrochloride	21111815	1
Euro OTC	Oxytetracycline hydrochloride	28011505	1
Euro OTC	Oxytetracycline hydrochloride	375-18	1
Euro OTC	Oxytetracycline hydrochloride	513E-02865	1
Euro OTC	Oxytetracycline hydrochloride	YT150502056	1
Euro OTC	Oxytetracycline hydrochloride	YT160702059	2
Euro OTC	Oxytetracycline hydrochloride	YT170302019	1
Euro/ Jenne	Oxytetracycline hydrochloride	1801033-01	1
Euro/Gehe	Oxytetracycline hydrochloride	1602025-02	1
Euro/Gehe	Oxytetracycline hydrochloride	170103	1
Euro/Gehe	Oxytetracycline hydrochloride	1701034-01	1
Euro/Gehe	Oxytetracycline hydrochloride	181033-02	1
Euro/Gehe	Oxytetracycline hydrochloride	2103010-01	2
Eurp OTG/AllianceHea...	Oxytetracycline hydrochloride	1801033-01	1
Fagro/Anzag	Oxytetracycline hydrochloride	14l22-B01-301464	1
Fagron	Oxytetracycline hydrochloride		1
Fagron	Oxytetracycline hydrochloride	12A26-N05	3
Fagron	Oxytetracycline hydrochloride	12G10-N04	7
Fagron	Oxytetracycline hydrochloride	130602203	1
Fagron	Oxytetracycline hydrochloride	13D08-N11	6
Fagron	Oxytetracycline hydrochloride	13I26-N11	1
Fagron	Oxytetracycline hydrochloride	13L19-B33	4
Fagron	Oxytetracycline hydrochloride	13L19-B33-290730	3
Fagron	Oxytetracycline hydrochloride	13L19-B33-290731	2
Fagron	Oxytetracycline hydrochloride	14/22-B01-301464	1
Fagron	Oxytetracycline hydrochloride	14/22-B01-301465	1
Fagron	Oxytetracycline hydrochloride	1407012-01	1
Fagron	Oxytetracycline hydrochloride	14I22-B01	1
Fagron	Oxytetracycline hydrochloride	14I22-B01-301464	1
Fagron	Oxytetracycline hydrochloride	14I22-B01-301465	1
Fagron	Oxytetracycline hydrochloride	14l22-B01-301463	1
Fagron	Oxytetracycline hydrochloride	15D29-B99-308608	1
Fagron	Oxytetracycline hydrochloride	15D29-B99-309066	1
Fagron	Oxytetracycline hydrochloride	15D29-B99-309067	1
Fagron	Oxytetracycline hydrochloride	15l16-b02-322907	1
Fagron	Oxytetracycline hydrochloride	15L16-B02-322907	1
Fagron	Oxytetracycline hydrochloride	15L16-B02-322908	1
Fagron	Oxytetracycline hydrochloride	1701034-02	1
Fagron	Oxytetracycline hydrochloride	1801033-01	1
Fagron	Oxytetracycline hydrochloride	4-49732A-2	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Oxytetracycline hydrochloride	912A-02865	1
Fagron	Oxytetracycline hydrochloride	C22H25CIN209	1
Fagropn	Oxytetracycline hydrochloride	13L19-B33-290731	1
Fiebig	Oxytetracycline hydrochloride	1801033-01	1
Finteler Apotheke	Oxytetracycline hydrochloride	1602025-02	2
Gehe amax	Oxytetracycline hydrochloride	1506037-02	3
Gehe amax	Oxytetracycline hydrochloride	150603737-03	1
Gehe amax	Oxytetracycline hydrochloride	1701034-02	1
Gehe amax	Oxytetracycline hydrochloride	1801033-01	1
Gehe amax	Oxytetracycline hydrochloride	4-48969A	1
Gehe	Oxytetracycline hydrochloride	1205028-01	1
Gehe	Oxytetracycline hydrochloride	12A26-N05	2
Gehe	Oxytetracycline hydrochloride	12g10-n04	1
Gehe	Oxytetracycline hydrochloride	1306022-02	1
Gehe	Oxytetracycline hydrochloride	1407012-03	1
Gehe	Oxytetracycline hydrochloride	1602025-02	3
GEHE	Oxytetracycline hydrochloride	1602025-02	1
GEHE	Oxytetracycline hydrochloride	1701034-01	1
Gehe	Oxytetracycline hydrochloride	1701034-02	1
Gehe	Oxytetracycline hydrochloride	17316805	1
Gehe	Oxytetracycline hydrochloride	1801033-01	3
Gehe	Oxytetracycline hydrochloride	1801033-02	1
Gehe	Oxytetracycline hydrochloride	2103010-01	1
Gehe	Oxytetracycline hydrochloride	2103010-03	1
Ichthyol-Gesellschaft	Oxytetracycline hydrochloride	1801033-01	2
L12	Oxytetracycline hydrochloride	12328107	1
L12	Oxytetracycline hydrochloride	16340610	1
L30	Oxytetracycline hydrochloride	1701034-02	1
Laborchemie Apolda/Phönix	Oxytetracycline hydrochloride	1506037-02	1
Nachprüfung vom 23.07.	Oxytetracycline hydrochloride	91618269	1
Norbrook Lab.Ltd.	Oxytetracycline hydrochloride	1506037-01	2
Norbrook/Gehe	Oxytetracycline hydrochloride	140701203	1
Noweda/Euro	Oxytetracycline hydrochloride	2103010-01	1
Noweda	Oxytetracycline hydrochloride	140701202	1
Noweda	Oxytetracycline hydrochloride	140701203	1
Noweda	Oxytetracycline hydrochloride	1701034-01	1
Noweda	Oxytetracycline hydrochloride	1701034-02	1
Noweda	Oxytetracycline hydrochloride	1801033-01	2
noweda	Oxytetracycline hydrochloride	2103010	1
Noweda	Oxytetracycline hydrochloride	2103010-01	1
Noweda	Oxytetracycline hydrochloride	2103010-03	3
Phoenix	Oxytetracycline hydrochloride	1602025-02	1
Phoenix	Oxytetracycline hydrochloride	17316817	1
Phoenix	Oxytetracycline hydrochloride	3036	1
Phönix Gotha	Oxytetracycline hydrochloride	1232814	1
Phönix Gotha	Oxytetracycline hydrochloride	1407012-02	1
Phönix	Oxytetracycline hydrochloride	1205028-01	1
Phönix	Oxytetracycline hydrochloride	1701034-02	1
Puren Pharma GmbH / ...	Oxytetracycline hydrochloride	17316816	1
Sanacorp Stralsund	Oxytetracycline hydrochloride	2103010-02	1
Sanacorp	Oxytetracycline hydrochloride	1701034-01	1
SANACORP	Oxytetracycline hydrochloride	1801033-02	1
Yangzhou Liberty Pha...	Oxytetracycline hydrochloride	1801033-01	1
Yangzhou Liberty Pharma	Oxytetracycline hydrochloride	1801033-02	2

- 235 053 spectra from 1515 *Apo-Ident* customers from a total of 49 095 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Oxytetracycline hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Oxytetracycline hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	740	0	152 222
Type B	0	240	0	201 844
Type C	0	976	38	235 053

The substance/substance group *Oxytetracycline hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1892 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	96.2525 % (> 95.9566 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20847	21999	29.19	120.45
20848	21836	26.65	103.19
21039	21600	15.41	187.15
21600	21600	0.00	187.80
21836	21836	0.00	109.06
21915	21836	63.44	103.72
21999	21999	0.00	140.93
22503	22503	0.00	138.66
22546	22546	0.00	131.77
22658	22658	0.00	129.33
22669	22669	0.00	131.96
22839	22669	36.39	133.97
22846	22669	15.20	131.61

continued on the next page

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23137	23137	0.00	146.58
23970	23137	37.98	146.47
25657	25657	0.00	169.72

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Pancreas powder**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20976-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Pancreas powder; Pancreatis pulvis

Special notes

When selecting the *Pancreas powder* substance/substance group, the following information is displayed to the user:

- Advice: Currently no longer available from major pharmaceutical manufacturers. Therefore, batch maintenance is currently not possible.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Pancreas powder	5	1	2

Second-stage model

For differentiation of the substance/substance group *Pancreas powder* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Pancreas powder* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Lactose monohydrate	58.33	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Pancreas powder* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Pancreas powder*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Pancreas powder	13118902	20976	40	1402190
Caelo	Pancreas powder	13395203	21481	60	20131218
Caelo	Pancreas powder	161397	22482	60	20160527*
Caelo	Pancreas powder	16139708	23757	40	20160527
Caelo	Pancreas powder	16139708	23758	40	20160527
Caelo	Pancreas powder	20002501001	25520	40	20200929

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 6 reference samples from the substance/substance group *Pancreas powder*. These

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 682 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Pancreas powder*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Pancreas powder	173226	23797	40

- 202 044 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 1 *Apo-Ident* customers from 2 batches from the substance/substance group *Pancreas powder*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Pancreas powder	17322602	1
Caelo	Pancreas powder	17322611	1

- 236 065 spectra from 1515 *Apo-Ident* customers from a total of 49 256 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Pancreas powder* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pancreas powder* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	40	0	202 044
Type C	0	2	0	236 065

The substance/substance group *Pancreas powder* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9013 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20976	20976	0.00	142.30
21481	22482	14.42	124.04
22482	22482	0.00	88.57
23757	22482	5.97	93.86
23758	22482	6.13	90.59
25520	22482	14.08	109.08

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Papaverine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20481-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Papaverine hydrochloride; Papaverini hydrochloridum

Special notes

When selecting the *Papaverine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Papaverine hydrochloride	5	3	15

Second-stage model

For differentiation of the substance/substance group *Papaverine hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Papaverine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Doxylamine hydrogen succinate	87.21	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Papaverine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Papaverine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Papaverine hydrochloride	13324310	21735	60	20130920
Caelo	Papaverine hydrochloride	123161	23054	40	20121127*
Caelo	Papaverine hydrochloride	180876	25614	40	20180328*
Caelo	Papaverine hydrochloride	22003603	26502	30	20221216*
Caelo	Papaverine hydrochloride	22003603	26502SI	20	20221216*
Gatt-Koller	Papaverine hydrochloride	21J01628	27096	30	20210907

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 220 spectra of 6 reference samples from the substance/substance group *Papaverine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 742 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 5 reference samples from the substance/substance group *Papaverine hydrochloride*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Papaverine hydrochloride	163159	23053	40
Caelo	Papaverine hydrochloride	16315911	23928	40
Caelo	Papaverine hydrochloride	23001264	26851	40
Caelo	Papaverine hydrochloride	23001264	26851SI	20
Gatt-Koller	Papaverine hydrochloride	21J01628	27096SI†	20

- 201 924 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 18 spectra from 11 *Apo-Ident* customers from 16 batches from the substance/substance group *Papaverine hydrochloride*.

- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
Caelo	Papaverine hydrochloride		1
Caelo	Papaverine hydrochloride	12166105	1
Caelo	Papaverine hydrochloride	12166112	1
Caelo	Papaverine hydrochloride	12316105	1
Caelo	Papaverine hydrochloride	13324307	1
Caelo	Papaverine hydrochloride	15160601	1
Caelo	Papaverine hydrochloride	15160608	2
Caelo	Papaverine hydrochloride	16315903	1
Caelo	Papaverine hydrochloride	16315907	1
Caelo	Papaverine hydrochloride	16315911	1
Caelo	Papaverine hydrochloride	17358802	1
Caelo	Papaverine hydrochloride	1817Q-02043	1
Fagron	Papaverine hydrochloride	21F07-B09	2
GATT-KOLLER/PHOENIX	Papaverine hydrochloride	2927/07131314	1
Phönix Gotha	Papaverine hydrochloride	12166101	1
Phönix Gotha	Papaverine hydrochloride	13324306	1

- 236 049 spectra from 1515 *Apo-Ident* customers from a total of 49 242 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Papaverine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Papaverine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	220	0	152 742
Type B	0	160	0	201 924
Type C	0	17	1	236 049

The substance/substance group *Papaverine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.2727 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21735	26502	18.29	138.12
23054	23054	0.00	138.59
25614	25614	0.00	137.58
26502	26502	0.00	137.35
27096	23054	8.34	139.99

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Paracetamol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20972-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Paracetamol; Paracetamolum

Special notes

When selecting the *Paracetamol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Paracetamol	10	9	81

Second-stage model

For differentiation of the substance/substance group *Paracetamol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Paracetamol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	118.24	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Paracetamol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Paracetamol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Paracetamol	15075706	22608	40	20150424
Caelo	Paracetamol	15075707	22822	40	20150424
Caelo	Paracetamol	191851	24889	40	20190827*
Caelo	Paracetamol	20001174	25629	40	20200624*
Caelo	Paracetamol	22002446	26370	40	20220818*
Caelo	Paracetamol	22002446	26370SI	20	20220818*
Euro OTC	Paracetamol	1111024-02	21598	60	20120123
Fagron	Paracetamol	13D30-N03	20972	40	1402271
Fagron	Paracetamol	13D16-N08	20973	40	1402296
Fagron	Paracetamol	13G23-N03	20974	40	1402297
Fagron	Paracetamol	21K05-B01-223625	26379	40	20220307
Fagron	Paracetamol	21K05-B01-223625	26379SI	20	20220307

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 460 spectra of 12 reference samples from the substance/substance group *Paracetamol*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 502 spectra from a total of 2832 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 400 spectra of 11 reference samples from the substance/substance group *Paracetamol*.

- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Paracetamol	170284	23852	40
Caelo	Paracetamol	180830	24053	40
Caelo	Paracetamol	22003365	26492	40
Caelo	Paracetamol	22003972	26497	40
Euro OTC	Paracetamol	2003059	25144	40
Euro OTC	Paracetamol	2211002	26426	40
Euro OTC	Paracetamol	2301037	26588	40
Euro OTC	Paracetamol	2301022	26597	40
Euro OTC	Paracetamol	2401012	27142	40
Caelo	Paracetamol	22003365	26492SI	20
Caelo	Paracetamol	22003972	26497SI	20

- 201 684 spectra from a total of 4036 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 212 spectra from 120 *Apo-Ident* customers from 83 batches from the substance/substance group *Paracetamol*.

- Among them are spectra of independent samples from 80 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Paracetamol	22002805001	1
	Paracetamol	22003365004	1
	Paracetamol	230102201	1
	Paracetamol	2301022-01	3
	Paracetamol	231022-01	1
Anzag	Paracetamol	22003972003	1
Caeleo/ Kehr	Paracetamol	19185102	4
Caeleo/ Kehr	Paracetamol	20003925002	3
Caelo	Paracetamol		1
Caelo	Paracetamol	10065102	1
Caelo	Paracetamol	10325020	1
Caelo	Paracetamol	11300108	1
Caelo	Paracetamol	11300120	2
Caelo	Paracetamol	13082005	1
Caelo	Paracetamol	13082010	3
Caelo	Paracetamol	13082011	1
Caelo	Paracetamol	15075704	4
Caelo	Paracetamol	15075708	1
Caelo	Paracetamol	15217701	1
Caelo	Paracetamol	15217704	1
Caelo	Paracetamol	15217706	1
Caelo	Paracetamol	15217708	1
Caelo	Paracetamol	15217710	5
Caelo	Paracetamol	15217712	2
Caelo	Paracetamol	15245901	3
Caelo	Paracetamol	15245902	1
Caelo	Paracetamol	17028409	4
Caelo	Paracetamol	17028411	3
Caelo	Paracetamol	18018602	1
Caelo	Paracetamol	18018604	1
Caelo	Paracetamol	18083003	4
Caelo	Paracetamol	18083005	5
Caelo	Paracetamol	18083006	4
Caelo	Paracetamol	18083007	1
Caelo	Paracetamol	18083012	2
Caelo	Paracetamol	18083014	5
Caelo	Paracetamol	1814U-02045	1
Caelo	Paracetamol	1912M-02045	1
Caelo	Paracetamol	191851001	1
Caelo	Paracetamol	191851002	2
Caelo	Paracetamol	191851004	6
Caelo	Paracetamol	20001174002	3
Caelo	Paracetamol	20003925001	1
Caelo	Paracetamol	20003925002	2
Caelo	Paracetamol	20003925004	5
Caelo	Paracetamol	20003925005	2
Caelo	Paracetamol	20003925007	2
Caelo	Paracetamol	20003925008	1
Caelo	Paracetamol	20003925009	1
Caelo	Paracetamol	20003925011	1
Caelo	Paracetamol	20003925014	1
Caelo	Paracetamol	20003925015	2
Caelo	Paracetamol	20003925016	2
Caelo	Paracetamol	20003925018	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Paracetamol	2000392504	1
Caelo	Paracetamol	2000395016	1
Caelo	Paracetamol	211222	1
Caelo	Paracetamol	22002446004	2
Caelo	Paracetamol	22002446005	3
Caelo	Paracetamol	22002805001	8
Caelo	Paracetamol	22002805005	1
Caelo	Paracetamol	22003365002	2
Caelo	Paracetamol	2815I-02045	1
Caelo	Paracetamol	5116I-02045	1
Caesar & Loretz GmbH...	Paracetamol	22002805002	2
Caesar & Loretz GmbH...	Paracetamol	22002805001	1
Caesar & Loretz GmbH...	Paracetamol	18083012	1
Caesar & Loretz GmbH/AHD	Paracetamol	22002446002	1
Caesar & Loretz GmbH/Gehe	Paracetamol	20003925009	1
Caesar & Loretz GmbH/Kehr	Paracetamol	22002805001	1
Caesar & Loretz GmbH...	Paracetamol	22002805007	1
Caesar & Loretz GmbH...	Paracetamol	20003925005	2
Caesar & Loretz GmbH...	Paracetamol	22002805002	1
Caesar & Loretz GmbH	Paracetamol	18083003	1
Caesar & Loretz GmbH	Paracetamol	18083006	1
Caesar & Loretz GmbH	Paracetamol	18083008	1
Caesar & Loretz GmbH	Paracetamol	191851002	2
Caesar & Loretz GmbH	Paracetamol	191851004	1
Caesar & Loretz GmbH	Paracetamol	20003925017	1
Caesar & Loretz GmbH	Paracetamol	22002446002	1
Caesar & Loretz GmbH	Paracetamol	22002446004	3
Caesar & Loretz GmbH	Paracetamol	22002446005	2
Caesar & Loretz GmbH	Paracetamol	22002805001	1
Caesar & Loretz GmbH	Paracetamol	22002805002	1
Caesar & Loretz GmbH	Paracetamol	22003365002	1
Caesar & Loretz GmbH	Paracetamol	22003365004	1
Caesar & Loretz GmbH	Paracetamol	22003365007	1
Caesar & Loretz Hilden	Paracetamol	18083006	1
Euro OTC	Paracetamol	1111024-01	1
Euro OTC	Paracetamol	1111024-02	1
Euro OTC	Paracetamol	17028409	1
Euro OTC	Paracetamol	2003059-01	3
Euro OTC	Paracetamol	2003059-02	1
Euro OTC	Paracetamol	2003059-03	3
Euro OTC	Paracetamol	200305904	2
Euro OTC	Paracetamol	2211002-01	5
Euro OTC	Paracetamol	2301022-01	1
Euro OTC	Paracetamol	3003059-02	1
Fagron	Paracetamol		1
Fagron	Paracetamol	13L16-B02-322725	1
Fagron	Paracetamol	17H17-B03	2
Fagron	Paracetamol	17H17-B03-359484	1
Fagron	Paracetamol	17H17-B03-367674	1
Fagron	Paracetamol	20F18-F02-224205	4
Fagron	Paracetamol	20F18-F02-374185	1
Gehe	Paracetamol	20003925007	1
Gehe	Paracetamol	2301022-01	1
Jenne	Paracetamol	15245901	1
Kehr	Paracetamol	20003925005	1
Nachprüfung	Paracetamol	15245901	2
Noweda	Paracetamol	18018602	2
Noweda	Paracetamol	2003059-02	1
Noweda	Paracetamol	20F18-F02-224205	1
Noweda	Paracetamol	2211002-01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Paracetamol	22002805001	1
Sanacorp	Paracetamol	22002805001	1

- 235 855 spectra from 1515 *Apo-Ident* customers from a total of 49 175 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Paracetamol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Paracetamol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	460	0	152 502
Type B	0	400	0	201 684
Type C	0	207	5	235 855

The substance/substance group *Paracetamol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6957 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.5000 %)
Type C	100.0000 % (> 99.9007 %)	97.6415 % (> 96.2264 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20972	20972	0.00	202.49
20973	20973	0.00	201.65
20974	20974	0.00	215.45
21598	24889	8.92	201.27

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22608	24889	7.60	199.11
22822	25629	8.23	202.96
24889	24889	0.00	207.78
25629	25629	0.00	205.86
26370	26370	0.00	203.62
26379	20974	26.25	215.84

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Patent blue V**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20469-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Patent blue V

Special notes

When selecting the *Patent blue V* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Patent blue V	6	2	15

Second-stage model

For differentiation of the substance/substance group *Patent blue V* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Patent blue V* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	55.34	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Patent blue V* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Patent blue V*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Patent blue V	12364206	21384	40	1508043
Caelo	Patent blue V	12364206	21385	40	20130110
Caelo	Patent blue V	13351803	21695	60	20131114
Caelo	Patent blue V	13351807	22387	40	1702362
Caelo	Patent blue V	190746	24731	40	20190425*
Caelo	Patent blue V	20000907	25212	40	20200604*
Caelo	Patent blue V	21002827	26118	40	20210923*
Caelo	Patent blue V	21002827	26118SI	20	20210923*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 320 spectra of 8 reference samples from the substance/substance group *Patent blue V*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Patent blue V*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Patent blue V	16306902	23214	40
Caelo	Patent blue V	22002332	26354	40
Caelo	Patent blue V	16306902	23215	40
Caelo	Patent blue V	22002332	26354SI	20

- 201 944 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 67 spectra from 58 *Apo-Ident* customers from 18 batches from the substance/substance group *Patent blue V*.

- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Patent blue V	22002332005	2
Bombastus	Patent blue V	11305302	1
Bombastus	Patent blue V	17034204	1
Caelo	Patent blue V	11305302	1
Caelo	Patent blue V	11305303	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Patent blue V	12364202	1
Caelo	Patent blue V	12364206	4
Caelo	Patent blue V	13351803	1
Caelo	Patent blue V	13351807	5
Caelo	Patent blue V	13351808	1
Caelo	Patent blue V	150602	1
Caelo	Patent blue V	15060204	2
Caelo	Patent blue V	16306904	4
Caelo	Patent blue V	17034204	8
Caelo	Patent blue V	17034207	6
Caelo	Patent blue V	17034210	4
Caelo	Patent blue V	19074603	8
Caelo	Patent blue V	20000907006	3
Caelo	Patent blue V	2759	1
Caelo	Patent blue V	P-15051823/17034204	1
Caesar & Loretz GmbH/Gehe	Patent blue V	19074603	1
Caesar & Loretz GmbH/Gehe	Patent blue V	20000907006	1
Caesar & Loretz GmbH	Patent blue V	17034207	1
Caesar & Loretz GmbH	Patent blue V	19074603	1
Caesar & Loretz GmbH	Patent blue V	20000907006	3
Euro OTC	Patent blue V	17034210	1
GEHE	Patent blue V	17034207	1

- 236 000 spectra from 1515 *Apo-Ident* customers from a total of 49 240 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Patent blue V* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Patent blue V* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	140	0	201 944
Type C	0	67	0	236 000

The substance/substance group *Patent blue V* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 91.0448 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21384	21384	0.00	150.30
21385	21384	3.70	148.79
21695	22387	6.43	132.68
22387	22387	0.00	136.11
24731	24731	0.00	92.77
25212	25212	0.00	86.82
26118	26118	0.00	99.83

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Pectin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10005975-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Pectin

Special notes

When selecting the *Pectin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Pectin	2	1	0

Second-stage model

For differentiation of the substance/substance group *Pectin* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Pectin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium dihydrogen phosphate dihydrate	60.71	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Pectin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Pectin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Pectin	21003677	26013	40	20220107*
Caelo	Pectin	24001504	27318	40	20240717*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Pectin*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 882 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 4 reference samples from the substance/substance group *Pectin*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Pectin	23000147	27108	40
Caelo	Pectin	21003677	26013SI†	10
Caelo	Pectin	23000147	27108SI	20
Caelo	Pectin	24001504	27318SI†	20

- 201 994 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Pectin*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Pectin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pectin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	80	0	152 882
Type B	0	90	0	201 994
Type C	0	0	0	236 067

The substance/substance group *Pectin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 93.3333 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26013	26013	0.00	96.35
27318	27318	0.00	89.43

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Phenazone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	22532-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Phenazone; Phenazonum

Special notes

When selecting the *Phenazone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Phenazone	7	4	4

Second-stage model

For differentiation of the substance/substance group *Phenazone* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Phenazone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Midazolam hydrochloride	99.95	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Phenazone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Phenazone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Phenazone	15415101	22576	40	20151215
Caelo	Phenazone	15415107	22827	40	20151215
Caelo	Phenazone	181347	24259	40	20180629*
Fagron	Phenazone	13G16-B07-287172	22532	40	AR-16-FG-011360-01
Fagron	Phenazone	13G16-B07-287172	22720	40	20130814
Fagron	Phenazone	15H28-B09-322944	24698	40	20150916
Fagron	Phenazone	21B23-B97-210607	25589	40	20210301
Fagron	Phenazone	22K28-B11-226183	26468	40	20221214
Fagron	Phenazone	22K28-B11-226183	26468SI	20	20221214

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 340 spectra of 9 reference samples from the substance/substance group *Phenazone*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 622 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 4 reference samples from the substance/substance group *Phenazone*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Phenazone	170836	23302	40
Caelo	Phenazone	182565	24369	40
Caelo	Phenazone	21002059	25797	50
Caelo	Phenazone	21003237	25847	50

- 201 904 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 4 *Apo-Ident* customers from 4 batches from the substance/substance group *Phenazone*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Phenazone	17083601	1
Caelo	Phenazone	18061101	1
Caelo	Phenazone	181347001	1
Caelo	Phenazone	182565002	1

- 236 063 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Phenazone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Phenazone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	340	0	152 622
Type B	0	180	0	201 904
Type C	0	4	0	236 063

The substance/substance group *Phenazone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2353 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22532	22532	0.00	199.58
22576	22532	10.93	198.97
22720	22532	3.10	200.93
22827	22532	9.09	199.00
24259	24259	0.00	196.72
24698	22532	17.72	200.48
25589	22532	16.61	202.44
26468	22532	15.96	207.63

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Pheniramine maleate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20694-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Pheniramine maleate; Pheniramini maleas

Special notes

When selecting the *Pheniramine maleate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Pheniramine maleate	6	5	41

Second-stage model

For differentiation of the substance/substance group *Pheniramine maleate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Pheniramine maleate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Dithranol	74.35	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Pheniramine maleate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Pheniramine maleate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Pheniramine maleate	12200502	20694	40	1401559
Caelo	Pheniramine maleate	15172702	22790	40	1908273
Euro OTC	Pheniramine maleate	1910024	24921	40	20191122*
Euro OTC	Pheniramine maleate	2209021	26348	40	20221018*
Euro OTC	Pheniramine maleate	2209021	26348SI	20	20221018*
Fagron	Pheniramine maleate	13D24-N04	20928	40	20130530
Fagron	Pheniramine maleate	18C21-B02-362029	24948	40	20180426

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 260 spectra of 7 reference samples from the substance/substance group *Pheniramine maleate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Pheniramine maleate*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Pheniramine maleate	173167	23821	40
Euro OTC	Pheniramine maleate	1109013-02	20756	40
Euro OTC	Pheniramine maleate	1701021	23384	40
Euro OTC	Pheniramine maleate	2304009	26640	40
Fagron	Pheniramine maleate	23B02-B03-222367	26668	40
Euro OTC	Pheniramine maleate	2304009	26640SI	20
Fagron	Pheniramine maleate	23B02-B03-222367	26668SI	20

- 201 844 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 96 spectra from 48 *Apo-Ident* customers from 42 batches from the substance/substance group *Pheniramine maleate*.

- Among them are spectra of independent samples from 41 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Pheniramine maleate	2209021-01	1
Alliance Healthcare	Pheniramine maleate	12L04-N05	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Anzag	Pheniramine maleate	17316706	2
Caelo	Pheniramine maleate	12352602	1
Caelo	Pheniramine maleate	12352604	1
Caelo	Pheniramine maleate	1235611	1
Caelo	Pheniramine maleate	14C25-B01-292540	1
Caelo	Pheniramine maleate	14C25-B01-302272	1
Caelo	Pheniramine maleate	14C25-B01-322989	1
Caelo	Pheniramine maleate	15172704	1
Caelo	Pheniramine maleate	15172708	1
Caelo	Pheniramine maleate	15172711	1
Caelo	Pheniramine maleate	173167001	1
Caelo	Pheniramine maleate	173167002	2
Caelo	Pheniramine maleate	173167003	1
Caelo	Pheniramine maleate	17316702	1
Caelo	Pheniramine maleate	17316705	1
Caelo	Pheniramine maleate	17316706	3
Caelo	Pheniramine maleate	17316707	1
Caelo	Pheniramine maleate	17316708	1
Caelo	Pheniramine maleate	9276210	1
Caesar & Loretz GmbH	Pheniramine maleate	173167002	6
Cealo	Pheniramine maleate	12352608	1
EuRO 14.11.2013 Phönix	Pheniramine maleate	1209032-01	1
Euro OTC	Pheniramine maleate	1109013-01	1
Euro OTC	Pheniramine maleate	1209032-01	2
Euro OTC	Pheniramine maleate	1411044-01	1
Euro OTC	Pheniramine maleate	1411044-02	3
Euro OTC	Pheniramine maleate	1701021-01	19
Euro OTC	Pheniramine maleate	1910024-01	1
Euro OTC	Pheniramine maleate	1910024-02	2
Euro OTC	Pheniramine maleate	2209021-01	2
Fagron	Pheniramine maleate	12I06-N02	1
Fagron	Pheniramine maleate	12L04-N05	3
Fagron	Pheniramine maleate	14C25-B01-292540	1
Fagron	Pheniramine maleate	14C25-B01-295293	3
Fagron	Pheniramine maleate	14c25b01307150	1
Fagron	Pheniramine maleate	14c25-b01-307150	1
Fagron	Pheniramine maleate	14C25-B01-307150	3
Fagron	Pheniramine maleate	14C25-B01-328732	2
Fagron	Pheniramine maleate	18C21-B02-351507	2
Fagron	Pheniramine maleate	18C21-B02-357417	1
Fagron	Pheniramine maleate	18C21-B02-369804	1
Fagron	Pheniramine maleate	18C21B02370926	1
Noweda 28.08.2019	Pheniramine maleate	15172714	1
Noweda	Pheniramine maleate	1701021	1
Sanacorp	Pheniramine maleate	18C21-B02-369804	1
Spangro_07.11.2018	Pheniramine maleate	1701021-01	7
Supriya LifeScience …	Pheniramine maleate	SLL/P/1213063	1
Supriya LifeScience …	Pheniramine maleate	14C25-B01	1

- 235 971 spectra from 1515 *Apo-Ident* customers from a total of 49 216 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Pheniramine maleate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

all relevant spectra of the various substances were compared with *Pheniramine maleate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	240	0	201 844
Type C	0	95	1	235 971

The substance/substance group *Pheniramine maleate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	98.9583 % (> 95.8333 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20694	20694	0.00	181.96
20928	20694	13.56	175.45
22790	22790	0.00	175.47
24921	24921	0.00	174.64
24948	22790	23.31	170.01
26348	26348	0.00	174.02

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Phenylbutazon**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20447-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Phenylbutazon; Phenylbutazonum

Special notes

When selecting the *Phenylbutazon* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Phenylbutazon	8	5	12

Second-stage model

For differentiation of the substance/substance group *Phenylbutazon* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Phenylbutazon* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Dithranol	126.01	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Phenylbutazon* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Phenylbutazon*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Phenylbutazon	14057202	21379	40	20140321
Caelo	Phenylbutazon	161121	22471	60	20160331*
Euro OTC	Phenylbutazon	1305050-02	21605	60	AR-15-FG-005687-01
Euro OTC	Phenylbutazon	1507023	21855	60	20150805*
Euro OTC	Phenylbutazon	1908013	24861	40	20190923*
Euro OTC	Phenylbutazon	2001046	25239	40	20200728*
Euro OTC	Phenylbutazon	2101032	25535	40	20210218*
Euro OTC	Phenylbutazon	2209001	26347	40	20220921*
Euro OTC	Phenylbutazon	2209001	26347SI	20	20220921*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 400 spectra of 9 reference samples from the substance/substance group *Phenylbutazon*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 562 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 220 spectra of 6 reference samples from the substance/substance group *Phenylbutazon*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Phenylbutazon	1604033	22563	40
Euro OTC	Phenylbutazon	1804018	24122	40
Euro OTC	Phenylbutazon	2107012	25830	50
Fagron	Phenylbutazon	18B21-B06-361114	24952	40
Fagron	Phenylbutazon	22G22-B03-221076	26451	40
Euro OTC	Phenylbutazon	2107012	25830SI	10

- 201 864 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 12 spectra from 11 *Apo-Ident* customers from 12 batches from the substance/substance group *Phenylbutazon*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Phenylbutazon	10262901	1
Caelo	Phenylbutazon	14099511	1
Caelo	Phenylbutazon	15218502	1
Caelo	Phenylbutazon	18063205	1
Euro OTC	Phenylbutazon	130505_01	1
Euro OTC	Phenylbutazon	170612PB/1604033-01	1
Euro OTC	Phenylbutazon	180401802	1
Euro OTC	Phenylbutazon	1804018-03	1
Euro OTC	Phenylbutazon	19091806	1
Euro OTC	Phenylbutazon	2001046-01	1
Fagron	Phenylbutazon	11H26-N02	1
Fagron	Phenylbutazon	13D30-N16	1

- 236 055 spectra from 1515 *Apo-Ident* customers from a total of 49 246 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Phenylbutazon* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Phenylbutazon* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	220	0	201 864
Type C	0	12	0	236 055

The substance/substance group *Phenylbutazon* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.2727 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21379	21605	5.19	217.82
21605	21605	0.00	212.75
21855	21855	0.00	216.16
22471	22471	0.00	214.78
24861	24861	0.00	222.53
25239	25239	0.00	222.13
25535	25535	0.00	224.70
26347	26347	0.00	224.54

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Phenylephrine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20567-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Phenylephrine hydrochloride; Phenylephrini hydrochloridum

Special notes

When selecting the *Phenylephrine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Phenylephrine hydrochloride	8	4	87

Second-stage model

For differentiation of the substance/substance group *Phenylephrine hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Phenylephrine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Caffeine citrate	129.54	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Phenylephrine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Phenylephrine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Phenylephrine hydrochloride	1704009	23394	40	20170524*
Euro OTC	Phenylephrine hydrochloride	2001012	25102	40	20200218*
Euro OTC	Phenylephrine hydrochloride	2109007	25823	50	20211006*
Euro OTC	Phenylephrine hydrochloride	2202012	26039	40	20220310*
Fagron	Phenylephrine hydrochloride	12J19-B40-288254	21051	40	20131210
Fagron	Phenylephrine hydrochloride	14H13-B02-308438	21960	60	AR-16-FG-008920-01
Fagron	Phenylephrine hydrochloride	16A20-B07-317987	22388	40	AR-16-FG-013385-01
Fagron	Phenylephrine hydrochloride	20D01-F06-370692	25366	40	20200529

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 350 spectra of 8 reference samples from the substance/substance group *Phenylephrine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 612 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 250 spectra of 7 reference samples from the substance/substance group *Phenylephrine hydrochloride*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Phenylephrine hydrochloride	2010018	25455	40
Fagron	Phenylephrine hydrochloride	17C23-B04-333878	23263	40
Fagron	Phenylephrine hydrochloride	17C23-B04-333880	23267	40
Fagron	Phenylephrine hydrochloride	22D28-B01-218602	26167	40
Euro OTC	Phenylephrine hydrochloride	2109007	25823SI†	10
Euro OTC	Phenylephrine hydrochloride	2202012	26039SI†	40
Fagron	Phenylephrine hydrochloride	22D28-B01-218602	26167SI	40

- 201 834 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 208 spectra from 38 *Apo-Ident* customers from 92 batches from the substance/substance group *Phenylephrine hydrochloride*.

- Among them are spectra of independent samples from 87 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Phenylephrine hydrochloride	21C04-F02-377267	1
	Phenylephrine hydrochloride	21F15-B10-216432	1
	Phenylephrine hydrochloride	23A04-B05-226165	1
ALH	Phenylephrine hydrochloride	16A20-B07-322159	1
Audor Pharma	Phenylephrine hydrochloride	APP70-16017PE	1
Audor Pharma	Phenylephrine hydrochloride	APP70-17001PE	2
Audor Pharma	Phenylephrine hydrochloride	APP70-17011PE	1
Audor Pharma	Phenylephrine hydrochloride	APP70-18008PE	1
Caelo	Phenylephrine hydrochloride	14H13-B02-308438	1
Caelo	Phenylephrine hydrochloride	17C23-B04-334819	1
Caelo	Phenylephrine hydrochloride	17H18-B02_353092	1
Caelo	Phenylephrine hydrochloride	17H18-B02-349261	2
Caelo	Phenylephrine hydrochloride	17H18-B02-353092	1
Caelo	Phenylephrine hydrochloride	18026008	1
Euro OTC	Phenylephrine hydrochloride	1704009-01	1
Euro OTC	Phenylephrine hydrochloride	2001012-01	1
Euro OTC	Phenylephrine hydrochloride	2010018-01	1
Euro OTC	Phenylephrine hydrochloride	21022182	1
Euro OTC	Phenylephrine hydrochloride	2109007-01	2
Fagon	Phenylephrine hydrochloride	20D01-F06-370690	1
Fagron	Phenylephrine hydrochloride	10091504	1
Fagron	Phenylephrine hydrochloride	1021402	1
Fagron	Phenylephrine hydrochloride	12031801	1
Fagron	Phenylephrine hydrochloride	12A03-N09	1
Fagron	Phenylephrine hydrochloride	12C08-N17	1
Fagron	Phenylephrine hydrochloride	12g19-n04	1
Fagron	Phenylephrine hydrochloride	12G19-N04	1
Fagron	Phenylephrine hydrochloride	12J19-B40-288253	2
Fagron	Phenylephrine hydrochloride	13A03-N09	3
Fagron	Phenylephrine hydrochloride	13B14-N03	1
Fagron	Phenylephrine hydrochloride	13G10-N04	1
Fagron	Phenylephrine hydrochloride	13K25-B02-293844	3
Fagron	Phenylephrine hydrochloride	13K25-B02-293845	1
Fagron	Phenylephrine hydrochloride	14H13-02-309892	1
Fagron	Phenylephrine hydrochloride	14H13-B02	1
Fagron	Phenylephrine hydrochloride	14H13-B02-299814	1
Fagron	Phenylephrine hydrochloride	14H13-B02-299816	2
Fagron	Phenylephrine hydrochloride	14H13B02299817	1
Fagron	Phenylephrine hydrochloride	14H13B02-299817	1
Fagron	Phenylephrine hydrochloride	14H13B02309892	1
Fagron	Phenylephrine hydrochloride	14H13-B02-309892	4
Fagron	Phenylephrine hydrochloride	15F09-B08-316796	2
Fagron	Phenylephrine hydrochloride	16A20-B07-233159	1
Fagron	Phenylephrine hydrochloride	16A20-B07-317987	2
Fagron	Phenylephrine hydrochloride	16A20B07322159	1
Fagron	Phenylephrine hydrochloride	16A20-B07-323398	3
Fagron	Phenylephrine hydrochloride	16A-B07-317987	1
Fagron	Phenylephrine hydrochloride	17C23-B04-333878	3
Fagron	Phenylephrine hydrochloride	17C23-B04-333879	1
Fagron	Phenylephrine hydrochloride	17c23-b04-333880	1
Fagron	Phenylephrine hydrochloride	17C23-B04-333880	1
Fagron	Phenylephrine hydrochloride	17C23-B04-334819	7
Fagron	Phenylephrine hydrochloride	17H18-B02	1
Fagron	Phenylephrine hydrochloride	17-H18-B02	1
Fagron	Phenylephrine hydrochloride	17H18-B02-345401	3
Fagron	Phenylephrine hydrochloride	17H18-B02-348065	1
Fagron	Phenylephrine hydrochloride	17H18-B02-349261	2
Fagron	Phenylephrine hydrochloride	17H18-B02-349262	4
Fagron	Phenylephrine hydrochloride	17H18-B02-353092	2
Fagron	Phenylephrine hydrochloride	17H-18-B02-353092	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Phenylephrine hydrochloride	17-H18-B02-353092	1
Fagron	Phenylephrine hydrochloride	17H18-B02-353093	1
Fagron	Phenylephrine hydrochloride	18L06-B02	8
Fagron	Phenylephrine hydrochloride	18L06-B02-360768	15
Fagron	Phenylephrine hydrochloride	18L06-B02-363037	2
Fagron	Phenylephrine hydrochloride	18L06-B02-367069	4
Fagron	Phenylephrine hydrochloride	18L06-B02-367673	11
Fagron	Phenylephrine hydrochloride	198099-0004	1
Fagron	Phenylephrine hydrochloride	19L06-B02-360768	1
Fagron	Phenylephrine hydrochloride	19L06-B02-367069	1
Fagron	Phenylephrine hydrochloride	20D01-F06	4
Fagron	Phenylephrine hydrochloride	20D01-F06-0003	1
Fagron	Phenylephrine hydrochloride	20D01-F06-370691	8
Fagron	Phenylephrine hydrochloride	20D01-F06-370692	1
Fagron	Phenylephrine hydrochloride	20D01-F06-373487	7
Fagron	Phenylephrine hydrochloride	20G10-F09	2
Fagron	Phenylephrine hydrochloride	20G10-F09-373759	1
Fagron	Phenylephrine hydrochloride	21C04-F02	1
Fagron	Phenylephrine hydrochloride	21C04-F02-377267	1
Fagron	Phenylephrine hydrochloride	21F15-B10	2
Fagron	Phenylephrine hydrochloride	21F15-B10-216432	1
Fagron	Phenylephrine hydrochloride	21F15-B10-217523	6
Fagron	Phenylephrine hydrochloride	2-IL-D-0080117	1
Fagron	Phenylephrine hydrochloride	B02-3670609	1
Fagron	Phenylephrine hydrochloride	B02-3676703	2
Fagron	Phenylephrine hydrochloride	F06-3706900	2
Fagron	Phenylephrine hydrochloride	F06-3706901	2
Fagron	Phenylephrine hydrochloride	F06-3706902	1
Fagron	Phenylephrine hydrochloride	PEH-170717	3
Fagron	Phenylephrine hydrochloride	PEH-200305	1
Gatt-Koller	Phenylephrine hydrochloride	330010164116	1
GEHE	Phenylephrine hydrochloride	17H18-B02	6
GEHE	Phenylephrine hydrochloride	17H18-B02-345401	2
GEHE	Phenylephrine hydrochloride	18L06-B02	3
Jenne	Phenylephrine hydrochloride	14H13-B02	2
JENNE	Phenylephrine hydrochloride	17H18-B02-339756	1
Nachprüfung	Phenylephrine hydrochloride	123456	1
Noweda/Fargon	Phenylephrine hydrochloride	17C23-B04-336301	4
Noweda	Phenylephrine hydrochloride	12F01-N20	2
Phoenix	Phenylephrine hydrochloride	15F09-B08	1
PHÖNIX	Phenylephrine hydrochloride	17C23-B04-334819	1

- 235 859 spectra from 1515 *Apo-Ident* customers from a total of 49 169 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Phenylephrine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Phenylephrine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	350	0	152 612
Type B	0	250	0	201 834
Type C	0	208	0	235 859

The substance/substance group *Phenylephrine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2857 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.6000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 97.1154 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21051	21960	5.12	299.50
21960	21960	0.00	299.90
22388	22388	0.00	300.33
23394	23394	0.00	298.06
25102	25102	0.00	302.86
25366	21960	5.75	301.39
25823	25823	0.00	291.47
26039	26039	0.00	288.00

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Phenytoin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20949-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Phenytoin; Phenytoinum

Special notes

When selecting the *Phenytoin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Phenytoin	5	3	3

Second-stage model

For differentiation of the substance/substance group *Phenytoin* the following second-stage model is used:

- Submodel 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Phenytoin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	106.70	–
⋮	⋮	⋮
Saccharin sodium	>50	86.00
Propranolol hydrochloride	>50	113.41
Quinoline yellow	>50	139.79
Atropine sulfate	>50	165.12
Mometasone furoate	>50	191.45
Magnesium hydrogen citrate	>50	254.17
Calcium orotate dihydrate	>50	262.23
Potassium sorbate	>50	371.26
Hydrocortisone	>50	398.03
Escin, water-soluble	>50	643.74

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Phenytoin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Phenytoin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Phenytoin	13G26-N02	20949	40	1401380
Fagron	Phenytoin	15E12-B05-312661	22271	45	20150519
Fagron	Phenytoin	18F01-B02-350492	24438	40	20180705
Fagron	Phenytoin	18F01-B02-350492	24693	40	20180705
Fagron	Phenytoin	19E14-B02	24818	40	20190722
Fagron	Phenytoin	22A17-F03-381312	27041	40	20220301

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 245 spectra of 6 reference samples from the substance/substance group *Phenytoin*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 717 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 5 reference samples from the substance/substance group *Phenytoin*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Phenytoin	12I07-N02	20678	40
Fagron	Phenytoin	16C14-B06-325086	23110	40
Fagron	Phenytoin	17L22-B04-345861	23994	40
Fagron	Phenytoin	16C14-B06-325086	23377	40
Fagron	Phenytoin	22A17-F03-381312	27041SI†	20

- 201 904 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Phenytoin*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Phenytoin	22A17-F03-381312	1
Caelo	Phenytoin	17L22-B04-345861	1
Fagron	Phenytoin	12C27N13	1
Fagron	Phenytoin	12I07-N02	1
Fagron	Phenytoin	13G26-N02	1
Fagron	Phenytoin	22A17-F03-381312	1

- 236 061 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Phenytoin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Phenytoin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	245	0	152 717
Type B	0	180	0	201 904
Type C	0	6	0	236 061

The substance/substance group *Phenytoin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5510 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20949	20949	0.00	316.53
22271	20949	18.03	316.71
24438	20949	7.96	316.10
24693	20949	5.49	317.74
24818	20949	7.07	316.55
27041	20949	24.64	309.94

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Pilocarpine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21519-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Pilocarpine hydrochloride; Pilocarpini hydrochloridum

Special notes

When selecting the *Pilocarpine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Pilocarpine hydrochloride	7	6	56

Second-stage model

For differentiation of the substance/substance group *Pilocarpine hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Pilocarpine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ofloxacin	52.17	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Pilocarpine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Pilocarpine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Pilocarpine hydrochloride	12217319	21518	60	20120806
Caelo	Pilocarpine hydrochloride	12217319	21519	60	1501660
Caelo	Pilocarpine hydrochloride	171595	23337	40	20170606*
Caelo	Pilocarpine hydrochloride	17124208	23371	40	20170607
Euro OTC	Pilocarpine hydrochloride	1305044-01	21629	60	20130725
Euro OTC	Pilocarpine hydrochloride	1305044-01	21629SI	60	20130725
Euro OTC	Pilocarpine hydrochloride	1603047	22553	40	20160429*
Euro OTC	Pilocarpine hydrochloride	1603047	22553SI	40	20160429*
Euro OTC	Pilocarpine hydrochloride	1908008	24845	40	20190830*
Fagron	Pilocarpine hydrochloride	22H16-B10-221817	26386	40	20220912
Fagron	Pilocarpine hydrochloride	22H16-B10-221817	26386SI	40	20220912

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 520 spectra of 11 reference samples from the substance/substance group *Pilocarpine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 442 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 660 spectra of 16 reference samples from the substance/substance group *Pilocarpine hydrochloride*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Pilocarpine hydrochloride	171242	23338	40
Caelo	Pilocarpine hydrochloride	191220	24762	40
Caelo	Pilocarpine hydrochloride	23000207	26727	40
Euro OTC	Pilocarpine hydrochloride	1806012	24140	40
Euro OTC	Pilocarpine hydrochloride	2010012	25478	40
Euro OTC	Pilocarpine hydrochloride	2208009	26270	40
Caelo	Pilocarpine hydrochloride	12217319	21518SI†	60
Caelo	Pilocarpine hydrochloride	171595	23337SI†	40
Caelo	Pilocarpine hydrochloride	171242	23338SI	40
Caelo	Pilocarpine hydrochloride	17124208	23371SI†	40
Caelo	Pilocarpine hydrochloride	191220	24762SI	40
Caelo	Pilocarpine hydrochloride	23000207	26727SI	40
Euro OTC	Pilocarpine hydrochloride	1806012	24140SI	40
Euro OTC	Pilocarpine hydrochloride	1908008	24845SI†	40
Euro OTC	Pilocarpine hydrochloride	2010012	25478SI	40
Euro OTC	Pilocarpine hydrochloride	2208009	26270SI	40

- 201 424 spectra from a total of 4035 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 189 spectra from 107 *Apo-Ident* customers from 60 batches from the substance/substance group *Pilocarpine hydrochloride*.
- Among them are spectra of independent samples from 56 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Pilocarpine hydrochloride	2208009-01	2
	Pilocarpine hydrochloride	23000207002	1
	Pilocarpine hydrochloride	24001858003	1
1806012-01	Pilocarpine hydrochloride	15198603	1
1Caesar & Loretz GmbH	Pilocarpine hydrochloride	21001750010	1
Caelo	Pilocarpine hydrochloride	11161903	1
Caelo	Pilocarpine hydrochloride	12217302	1
Caelo	Pilocarpine hydrochloride	12217307	1
Caelo	Pilocarpine hydrochloride	12217316	1
Caelo	Pilocarpine hydrochloride	12K07-N09	1
Caelo	Pilocarpine hydrochloride	130504401	1
Caelo	Pilocarpine hydrochloride	1305044-03	1
Caelo	Pilocarpine hydrochloride	14239402	1
Caelo	Pilocarpine hydrochloride	15198610	2
Caelo	Pilocarpine hydrochloride	15198701	2
Caelo	Pilocarpine hydrochloride	1603047-02	3
Caelo	Pilocarpine hydrochloride	17124208	4
Caelo	Pilocarpine hydrochloride	17159510	1
Caelo	Pilocarpine hydrochloride	17236401	1
Caelo	Pilocarpine hydrochloride	17332002	4
Caelo	Pilocarpine hydrochloride	18138704	6
Caelo	Pilocarpine hydrochloride	18138709	1
Caelo	Pilocarpine hydrochloride	191220001	5
Caelo	Pilocarpine hydrochloride	19122001	1
Caelo	Pilocarpine hydrochloride	21000139001	2
Caelo	Pilocarpine hydrochloride	21001750003	4
Caelo	Pilocarpine hydrochloride	2211112032607	1
Caelo	Pilocarpine hydrochloride	25051303	1
Caesar & Loretz GmbH...	Pilocarpine hydrochloride	191220001	1
Caesar & Loretz GmbH...	Pilocarpine hydrochloride	191220001	1
Caesar & Loretz GmbH...	Pilocarpine hydrochloride	191220009	4
Caesar & Loretz GmbH...	Pilocarpine hydrochloride	191220001	1
Caesar & Loretz GmbH	Pilocarpine hydrochloride	191220001	1
Caesar & Loretz GmbH	Pilocarpine hydrochloride	191220003	1
Caesar & Loretz GmbH	Pilocarpine hydrochloride	19122001	1
Caesar & Loretz GmbH	Pilocarpine hydrochloride	21000139001	1
Caesar & Loretz GmbH	Pilocarpine hydrochloride	21000139002	3
Caesar & Loretz GmbH	Pilocarpine hydrochloride	21000139005	4
Caesar & Loretz GmbH	Pilocarpine hydrochloride	21001750003	4
EuRho/Noweda	Pilocarpine hydrochloride	18060012-01	1
Euro OTC	Pilocarpine hydrochloride	1202031-01	1
Euro OTC	Pilocarpine hydrochloride	1202031-02	1
Euro OTC	Pilocarpine hydrochloride	13050-14-01	1
Euro OTC	Pilocarpine hydrochloride	130504401	2
Euro OTC	Pilocarpine hydrochloride	1305044-01	6
Euro OTC	Pilocarpine hydrochloride	1305044-03	2
Euro OTC	Pilocarpine hydrochloride	1603047	1
Euro OTC	Pilocarpine hydrochloride	1603047-01	6
Euro OTC	Pilocarpine hydrochloride	160304702	1
Euro OTC	Pilocarpine hydrochloride	1603047-02	28

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Pilocarpine hydrochloride	1806012-01	12
Euro OTC	Pilocarpine hydrochloride	1806012-02	4
Euro OTC	Pilocarpine hydrochloride	18CB02	1
Euro OTC	Pilocarpine hydrochloride	19008008-01	1
Euro OTC	Pilocarpine hydrochloride	190800	1
Euro OTC	Pilocarpine hydrochloride	1908008-01	16
Euro OTC	Pilocarpine hydrochloride	19CC02	1
Euro OTC	Pilocarpine hydrochloride	2010012-01	4
Euro OTC	Pilocarpine hydrochloride	Euroo	1
Euro OTG	Pilocarpine hydrochloride	1305044-01	1
Fagron	Pilocarpine hydrochloride	13H24-N03	1
Fagron	Pilocarpine hydrochloride	15B27-B03-309493	1
Fagron	Pilocarpine hydrochloride	18A31-B05-346072	1
Fagron	Pilocarpine hydrochloride	18A31-B05350799	1
Fagron	Pilocarpine hydrochloride	18A31-B05-350799	6
Fagron	Pilocarpine hydrochloride	19E20-B13-191235	1
Fagron	Pilocarpine hydrochloride	20D14-B05-196754	2
Fagron	Pilocarpine hydrochloride	20H18-B06-203134	1
Fagron	Pilocarpine hydrochloride	350799	1
Gehe	Pilocarpine hydrochloride	15198610	1
Gehe	Pilocarpine hydrochloride	17124209	1
Gehe	Pilocarpine hydrochloride	1806012-02	1
GEHE	Pilocarpine hydrochloride	18138704	1
Leyhs	Pilocarpine hydrochloride	15198701	1
Phönix	Pilocarpine hydrochloride	1603047-02	1
Sanacorp	Pilocarpine hydrochloride	12217302	1
SourcetechQuimica/Noweda	Pilocarpine hydrochloride		1

- 235 878 spectra from 1515 *Apo-Ident* customers from a total of 49 199 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Pilocarpine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pilocarpine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	520	0	152 442
Type B	0	660	0	201 424
Type C	0	189	0	235 878

The substance/substance group *Pilocarpine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8462 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0909 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 96.8254 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21518	24845	23.47	57.54
21519	21519	0.00	62.23
21629	24845	6.40	61.55
22553	22553	0.00	65.55
23337	23337	0.00	67.49
23371	21519	7.15	61.48
24845	24845	0.00	61.91
26386	21519	30.59	73.32

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Poloxamers**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20540-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Poloxamers; Poloxamera

Special notes

When selecting the *Poloxamers* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Poloxamers	6	6	46

Second-stage model

For differentiation of the substance/substance group *Poloxamers* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Poloxamers* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Glycerol monostearate, emulsifying	96.55	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Poloxamers* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Poloxamers*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Poloxamers	14196101	21652	60	AR-14-FG-013090-01
Caelo	Poloxamers	16242605	23257	40	20160915
Caelo	Poloxamers	20003669003	25509	40	20201117
Caelo	Poloxamers	22003362006	26746	40	20230208
Caelo	Poloxamers	22003362006	26746SI	20	20230208
Caelo	Poloxamers	23001663	27115	40	20231207*
Caelo	Poloxamers	23001663	27115SI	20	20231207*
Fagron	Poloxamers	14G17-B03-296866	21726	60	20140806

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 320 spectra of 8 reference samples from the substance/substance group *Poloxamers*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 250 spectra of 7 reference samples from the substance/substance group *Poloxamers*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Poloxamers	170486	23311	40
Caelo	Poloxamers	172921	23810	40
Caelo	Poloxamers	181607	24219	40
Caelo	Poloxamers	182636	24358	40
Caelo	Poloxamers	21001523004	25980	40
Caelo	Poloxamers	24002242	27437	40
Caelo	Poloxamers	21001523004	25980SI	10

- 201 834 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 136 spectra from 89 *Apo-Ident* customers from 50 batches from the substance/substance group *Poloxamers*.

- Among them are spectra of independent samples from 46 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Poloxamers	22003362006	1
	Poloxamers	22003362007	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
	Poloxamers	22003362010	1
Anzag	Poloxamers	22003362006	1
Caelo	Poloxamers	12286801	2
Caelo	Poloxamers	12286805	1
Caelo	Poloxamers	12286806	1
Caelo	Poloxamers	13133201	1
Caelo	Poloxamers	13133203	2
Caelo	Poloxamers	13133207	1
Caelo	Poloxamers	14196101	2
Caelo	Poloxamers	14196104	1
Caelo	Poloxamers	14196105	1
Caelo	Poloxamers	14196108	2
Caelo	Poloxamers	14359501	1
Caelo	Poloxamers	15183102	2
Caelo	Poloxamers	15397802	5
Caelo	Poloxamers	16189301	1
Caelo	Poloxamers	16189302	4
Caelo	Poloxamers	16242601	3
Caelo	Poloxamers	16242605	3
Caelo	Poloxamers	162426056	1
Caelo	Poloxamers	17048601	4
Caelo	Poloxamers	17048606	2
Caelo	Poloxamers	17292101	2
Caelo	Poloxamers	18025101	13
Caelo	Poloxamers	18160702	10
Caelo	Poloxamers	18160704	4
Caelo	Poloxamers	182636001	3
Caelo	Poloxamers	18263601	4
Caelo	Poloxamers	18263605	3
Caelo	Poloxamers	18263607	4
Caelo	Poloxamers	20000294001	3
Caelo	Poloxamers	20003669003	8
Caelo	Poloxamers	21001523001	4
Caelo	Poloxamers	22003362002	1
Caesar & Loretz GmbH…	Poloxamers	18263601	1
Caesar & Loretz GmbH/Gehe	Poloxamers	18263607	1
Caesar & Loretz GmbH…	Poloxamers	182636	1
Caesar & Loretz GmbH	Poloxamers	15183102	1
Caesar & Loretz GmbH	Poloxamers	182636002	3
Caesar & Loretz GmbH	Poloxamers	18263601	1
Caesar & Loretz GmbH	Poloxamers	18263607	1
Caesar & Loretz GmbH	Poloxamers	20000294001	1
Caesar & Loretz GmbH	Poloxamers	20003669003	2
Caesar & Loretz GmbH	Poloxamers	21001523001	1
Caesar & Loretz GmbH	Poloxamers	21001523004	2
Euro OTC	Poloxamers	15397802	1
Fagron	Poloxamers	12K23-N03	1
Fagron	Poloxamers	13G29-N01	1
Fagron	Poloxamers	13G29-NO1	1
Fagron	Poloxamers	15A26-B03-303503	1
Fagron	Poloxamers	315E-07027	1
Fagron	Poloxamers	318A-07027	1
Fagron	Poloxamers	5211Q-07027	1
Fagron	Poloxamers	5315I-07027	1
Fagron	Poloxamers	914I-07027	1
Fagron	Poloxamers	WPWI610C	1
Noweda	Poloxamers	18263607	1
Phonix	Poloxamers	12/13-N10	1
Sanacorp	Poloxamers	14196101	2
Sigma-Aldrich	Poloxamers	BCBW9875	1

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 235 931 spectra from 1515 *Apo-Ident* customers from a total of 49 208 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Poloxamers* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Poloxamers* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	250	0	201 834
Type C	0	135	1	235 931

The substance/substance group *Poloxamers* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.6000 %)
Type C	100.0000 % (> 99.9007 %)	99.2647 % (> 97.0588 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21652	21652	0.00	128.26
21726	21652	6.54	128.12
23257	21652	8.83	129.34
25509	27115	11.88	130.40
26746	21652	16.89	130.73
27115	27115	0.00	130.17

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Polymyxin B sulfate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20853-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Polymyxin B sulfate; Polymyxin B sulphate; Polymyxini B sulfas

Special notes

When selecting the *Polymyxin B sulfate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Polymyxin B sulfate	14	14	80

Second-stage model

For differentiation of the substance/substance group *Polymyxin B sulfate* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Polymyxin B sulfate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Colistin sulfate	40.74	18.66
Bacitracin	46.53	19.73
Calcium pantothenate	60.05	19.84
⋮	⋮	⋮
Riboflavin	>50	33.80
Amphotericin B	>50	41.16
Nystatin	>50	52.81
Cyanocobalamin	>50	56.42
Triamcinolone	>50	62.28
Methylcobalamin	>50	65.85
alpha-tocopheryl acetate dry concentrate	>50	75.82
Calcium glycerophosphate	>50	77.34
Gelatine, white	>50	79.09
Selenium yeast	>50	84.03
Estradiol hemihydrate	>50	86.68
Estriol	>50	90.55
Hyoscine hydrobromide	>50	100.16
Carmellose sodium	>50	119.76
Tosylchloramide sodium	>50	120.97
SyrSpend® SF Alka	>50	136.66
SyrSpend® SF pH4 neo (Maize starch)	>50	159.66
Rice starch	>50	166.04
Oxalic acid	>50	236.51
Corn starch	>50	243.23
Acacia, dried dispersion	>50	261.59
SyrSpend® SF pH4	>50	286.90
Potato starch	>50	339.84
Wheat starch	>50	347.00
Maltodextrin	>50	373.01
Fructose	>50	395.71

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Polymyxin B sulfate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Polymyxin B sulfate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Polymyxin B sulfate	153501	22451	60	20160318*
Caelo	Polymyxin B sulfate	181154	24407	40	20180507*
Euro OTC	Polymyxin B sulfate	1304033-01	21094	40	20130829
Euro OTC	Polymyxin B sulfate	1202039-02	21329	40	1411033
Euro OTC	Polymyxin B sulfate	1304033-02	21584	60	20130612
Euro OTC	Polymyxin B sulfate	1505005-01	21980	60	AR-16-FG-005387-01
Euro OTC	Polymyxin B sulfate	1604016	22542	40	20160509*
Euro OTC	Polymyxin B sulfate	2101014	25597	40	20210331*
Euro OTC	Polymyxin B sulfate	2303014	26763	40	20230525*
Fagron	Polymyxin B sulfate	13C12-N02	20853	40	1402691
Fagron	Polymyxin B sulfate	12G13-N05	21258	40	1410347
Fagron	Polymyxin B sulfate	13I13-N05	21595	45	AR-15-FG-001516-01
Fagron	Polymyxin B sulfate	14F04-B03-296722	21957	60	20140708
Fagron	Polymyxin B sulfate	15H14-B01-314364	22323	60	20150902

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 665 spectra of 14 reference samples from the substance/substance group *Polymyxin B sulfate*. These samples are listed above in the *calibration samples* section. The reference samples come from 14 different batches.
- 152 297 spectra from a total of 2828 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 660 spectra of 18 reference samples from the substance/substance group *Polymyxin B sulfate*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Polymyxin B sulfate	191131	24752	40
Caelo	Polymyxin B sulfate	22001497	26255	40
Caelo	Polymyxin B sulfate	23001927	26970	40
Euro OTC	Polymyxin B sulfate	1701010	23012	40
Euro OTC	Polymyxin B sulfate	1707013	23554	40
Euro OTC	Polymyxin B sulfate	1802006	23953	40
Euro OTC	Polymyxin B sulfate	1807004	24143	40
Euro OTC	Polymyxin B sulfate	1811022	24494	40
Euro OTC	Polymyxin B sulfate	1906002	24779	40
Euro OTC	Polymyxin B sulfate	1911021	25088	40
Euro OTC	Polymyxin B sulfate	2006009	25317	40
Euro OTC	Polymyxin B sulfate	2205005	26226	40
Fagron	Polymyxin B sulfate	13E06-N12	20912	40
Fagron	Polymyxin B sulfate	22A21-B03-218149	26144	40
Caelo	Polymyxin B sulfate	22001497	26255SI	20
Euro OTC	Polymyxin B sulfate	1202039-02	20904	40
Euro OTC	Polymyxin B sulfate	2205005	26226SI	20
Fagron	Polymyxin B sulfate	22A21-B03-218149	26144SI	20

- 201 424 spectra from a total of 4030 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 248 spectra from 161 *Apo-Ident* customers from 86 batches from the substance/substance group *Polymyxin B sulfate*.

- Among them are spectra of independent samples from 80 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Polymyxin B sulfate	2101014-01	1
	Polymyxin B sulfate	22K22-B02-224472	1
	Polymyxin B sulfate	230035622001	1
	Polymyxin B sulfate	2303014-01	2
	Polymyxin B sulfate	230314-01	1
Alliance Healthcare	Polymyxin B sulfate	1202039-02	1
apo-ident/Gehe/24,50	Polymyxin B sulfate	1807004-01	1
Biotika / Ebert	Polymyxin B sulfate	15011	1
Biotika a.s./Phoenix	Polymyxin B sulfate	2101014-01	1
Biotika/Noweda	Polymyxin B sulfate	200317	1
Biotika	Polymyxin B sulfate	150828	1
Bombastus	Polymyxin B sulfate	1604016-02	1
Caelo	Polymyxin B sulfate	1102013-01	1
Caelo	Polymyxin B sulfate	12G13-N05	3
Caelo	Polymyxin B sulfate	13H28-B02-287953	1
Caelo	Polymyxin B sulfate	150725	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Polymyxin B sulfate	15350101	8
Caelo	Polymyxin B sulfate	15350101P-190311-3	1
Caelo	Polymyxin B sulfate	1604016-01	3
Caelo	Polymyxin B sulfate	16C01-B04-319432	1
Caelo	Polymyxin B sulfate	170101001	3
Caelo	Polymyxin B sulfate	1701010-01	1
Caelo	Polymyxin B sulfate	1707013-01	1
Caelo	Polymyxin B sulfate	1802006-01	2
Caelo	Polymyxin B sulfate	1802006-011	1
Caelo	Polymyxin B sulfate	18115406	2
Caelo	Polymyxin B sulfate	18115410	2
Caelo	Polymyxin B sulfate	19113102	1
Caelo	Polymyxin B sulfate	19113103	1
Caelo	Polymyxin B sulfate	20003057003	3
Caesar & Loretz GmbH	Polymyxin B sulfate	20003057003	2
cealo	Polymyxin B sulfate	16c01-b04-319432	1
EuRho/Phoenix	Polymyxin B sulfate	2006009-01	1
EuRho	Polymyxin B sulfate	1202039-01	1
EuRho	Polymyxin B sulfate	1807004-01	1
EuRho	Polymyxin B sulfate	2006008-01	1
Euro OTC	Polymyxin B sulfate	11091419	1
Euro OTC	Polymyxin B sulfate	1202039-01	1
Euro OTC	Polymyxin B sulfate	1202039-02	4
Euro OTC	Polymyxin B sulfate	1304033-01	1
Euro OTC	Polymyxin B sulfate	1304033-02	1
Euro OTC	Polymyxin B sulfate	1304033-03	2
Euro OTC	Polymyxin B sulfate	1406012-01	3
Euro OTC	Polymyxin B sulfate	140601202	3
Euro OTC	Polymyxin B sulfate	1406012-02	5
Euro OTC	Polymyxin B sulfate	150500501	1
Euro OTC	Polymyxin B sulfate	1505005-01	6
Euro OTC	Polymyxin B sulfate	1505505-01	1
Euro OTC	Polymyxin B sulfate	1604016-01	2
Euro OTC	Polymyxin B sulfate	1604016-02	6
Euro OTC	Polymyxin B sulfate	170101001	1
Euro OTC	Polymyxin B sulfate	1701010-01	13
Euro OTC	Polymyxin B sulfate	1707013-01	10
Euro OTC	Polymyxin B sulfate	180200601	1
Euro OTC	Polymyxin B sulfate	1802006-01	8
Euro OTC	Polymyxin B sulfate	1807004-01	6
Euro OTC	Polymyxin B sulfate	1811022-01	7
Euro OTC	Polymyxin B sulfate	1906002-01	6
Euro OTC	Polymyxin B sulfate	1911021-01	5
Euro OTC	Polymyxin B sulfate	2006009-01	15
Euro OTC	Polymyxin B sulfate	2101014-01	21
Euro OTC	Polymyxin B sulfate	2205005-01	1
Euro OTC	Polymyxin B sulfate	23051502	1
Euro OTC	Polymyxin B sulfate	25101201	1
Euro OTC	Polymyxin B sulfate	28041730	1
Euroo/Phoenix	Polymyxin B sulfate	1304033-02	1
Fagron	Polymyxin B sulfate	12G13N05	1
Fagron	Polymyxin B sulfate	12G13-N05	1
Fagron	Polymyxin B sulfate	13/13-N05	1
Fagron	Polymyxin B sulfate	13G05-N06	2
Fagron	Polymyxin B sulfate	13H28-B02-287954	1
Fagron	Polymyxin B sulfate	13H28-B02-293470	1
Fagron	Polymyxin B sulfate	140822	1
Fagron	Polymyxin B sulfate	14F04-B03-296721	1
Fagron	Polymyxin B sulfate	14H12-B06-304727	1
Fagron	Polymyxin B sulfate	15H14-B01-315692	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Polymyxin B sulfate	16C01-B04	1
Fagron	Polymyxin B sulfate	16C01-B04-319432	1
Fagron	Polymyxin B sulfate	16c01b04322012	1
Fagron	Polymyxin B sulfate	16C01-B04-322012	3
Fagron	Polymyxin B sulfate	16G21-B03-333808	1
Fagron	Polymyxin B sulfate	170621	1
Fagron	Polymyxin B sulfate	17H23-B01-344840	2
Fagron	Polymyxin B sulfate	18B28B04351511	1
Fagron	Polymyxin B sulfate	18B28-B04-355722	2
Fagron	Polymyxin B sulfate	19/11-F01-368351	1
Fagron	Polymyxin B sulfate	191057	1
Fagron	Polymyxin B sulfate	19A23-B01-361158	4
Fagron	Polymyxin B sulfate	19A23-B01-3621201	1
Fagron	Polymyxin B sulfate	19A23-B01-362121	2
Fagron	Polymyxin B sulfate	19I11-F01-3683501	1
Fagron	Polymyxin B sulfate	20B21-F08-373930	1
Fagron	Polymyxin B sulfate	20F23-F01	1
Fagron	Polymyxin B sulfate	21K09-B10-213615	1
Fagron	Polymyxin B sulfate	22A21-B03-218149	1
Fagron	Polymyxin B sulfate	2517M-03315	1
Fagron	Polymyxin B sulfate	3518A-03315	1
Fagron	Polymyxin B sulfate	912A-03315	1
Fagron	Polymyxin B sulfate	F08-3739300	1
Fargon/Phoenix	Polymyxin B sulfate	17H23-B01-344840	1
Fiebig	Polymyxin B sulfate	1807004-01	1
Gatt-Koller	Polymyxin B sulfate	17H23B01344840	1
Gehe	Polymyxin B sulfate	170101001	1
GEHE	Polymyxin B sulfate	1701010-01	1
Noweda 03.08.2019	Polymyxin B sulfate	18115406	1
Phoenix	Polymyxin B sulfate	1807004-01	1
Phoenix	Polymyxin B sulfate	2006009-01	1
Phönix/Euro	Polymyxin B sulfate	1505005-010	1
Phönix	Polymyxin B sulfate	1202039-01	1
Phönix	Polymyxin B sulfate	1701010-01	1
Phönix	Polymyxin B sulfate	1707013	1
Rondell Apotheke	Polymyxin B sulfate	121161	1
Sanacorp	Polymyxin B sulfate	1707013-01	1
Sanacorp	Polymyxin B sulfate	2101014-01	1

- 235 819 spectra from 1515 *Apo-Ident* customers from a total of 49 174 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Polymyxin B sulfate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Polymyxin B sulfate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	665	0	152 297
Type B	0	660	0	201 424
Type C	0	244	4	235 819

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The substance/substance group *Polymyxin B sulfate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0977 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0909 %)
Type C	100.0000 % (> 99.9007 %)	98.3871 % (> 97.1774 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20853	20853	0.00	49.22
21094	21980	7.02	55.80
21258	21258	0.00	48.52
21329	21329	0.00	51.58
21584	21980	13.37	57.97
21595	21595	0.00	65.96
21957	22451	4.74	62.77
21980	21980	0.00	57.87
22323	25597	8.21	61.24
22451	22451	0.00	66.25
22542	22542	0.00	49.29
24407	24407	0.00	46.53
25597	25597	0.00	59.91
26763	26763	0.00	55.61

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Potassium citrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20021-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Potassium citrate; Kalii citras

Special notes

When selecting the *Potassium citrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Potassium citrate	11	14	171

Second-stage model

For differentiation of the substance/substance group *Potassium citrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Potassium citrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	86.37	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Potassium citrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Potassium citrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Potassium citrate	11320212	20655	40	20111201
Caelo	Potassium citrate	13317618	21452	60	20130926
Caelo	Potassium citrate	15123103	21775	60	20150414
Caelo	Potassium citrate	161130	22476	60	20160602*
Caelo	Potassium citrate	21000107	25558	40	20210113*
Caelo	Potassium citrate	22002808	26481	40	20221104*
Caelo	Potassium citrate	22002808	26481SI	20	20221104*
Euro OTC	Potassium citrate	1509044	21936	60	20151013*
Euro OTC	Potassium citrate	1611017	22921	40	20161207*
Euro OTC	Potassium citrate	1912008	25090	40	20200115*
Euro OTC	Potassium citrate	2101026	25607	40	20210126*
Euro OTC	Potassium citrate	2105012	25703	50	20210630*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 550 spectra of 12 reference samples from the substance/substance group *Potassium citrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 412 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 600 spectra of 16 reference samples from the substance/substance group *Potassium citrate*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Potassium citrate	170929	23290	40
Caelo	Potassium citrate	180385	24046	40
Caelo	Potassium citrate	191804	24736	40
Euro OTC	Potassium citrate	1603040	22521	40
Euro OTC	Potassium citrate	1606041	22676	40
Euro OTC	Potassium citrate	1705024	23428	40
Euro OTC	Potassium citrate	1803003	24084	40
Euro OTC	Potassium citrate	1807034	24160	40
Euro OTC	Potassium citrate	1902027	24485	40
Euro OTC	Potassium citrate	1907016	24785	40
Euro OTC	Potassium citrate	2008015	25346	40
Euro OTC	Potassium citrate	2109025	25881	50
Euro OTC	Potassium citrate	2212005	26535	40
Euro OTC	Potassium citrate	2311001	27006	40
Euro OTC	Potassium citrate	2109025	25881SI	10
Euro OTC	Potassium citrate	2212005	26535SI	20

- 201 484 spectra from a total of 4031 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 522 spectra from 232 *Apo-Ident* customers from 177 batches from the substance/substance group *Potassium citrate*.
- Among them are spectra of independent samples from 171 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Potassium citrate		1
	Potassium citrate	123345	1
	Potassium citrate	12345	1
	Potassium citrate	22002808006	1
	Potassium citrate	2212005-01	5
	Potassium citrate	24000093002	1
	Potassium citrate	24000093005	1
	Potassium citrate	hfdf5545	1
ACM	Potassium citrate	KNC0196J15	4
Alliance/EurRho	Potassium citrate	3055187	1
Alliance	Potassium citrate	1611017-01	1
Caelo	Potassium citrate		9
Caelo	Potassium citrate	11102201	1
Caelo	Potassium citrate	1112008-01	1
Caelo	Potassium citrate	11320201	1
Caelo	Potassium citrate	11320212	3
Caelo	Potassium citrate	116I-01737	1
Caelo	Potassium citrate	1204016-01	1
Caelo	Potassium citrate	12135302	6
Caelo	Potassium citrate	12135303	2
Caelo	Potassium citrate	12135309	2
Caelo	Potassium citrate	12135311	1
Caelo	Potassium citrate	1215309	1
Caelo	Potassium citrate	12299201	5
Caelo	Potassium citrate	12299202	1
Caelo	Potassium citrate	12299203	4
Caelo	Potassium citrate	12334	1
Caelo	Potassium citrate	1234	4
Caelo	Potassium citrate	12345	3
Caelo	Potassium citrate	12345678	1
Caelo	Potassium citrate	123654879	1
Caelo	Potassium citrate	123test	2
Caelo	Potassium citrate	123Test	4
Caelo	Potassium citrate	123Testmessung	1
Caelo	Potassium citrate	12456	1
Caelo	Potassium citrate	1256369	1
Caelo	Potassium citrate	12648	1
Caelo	Potassium citrate	13080602	8
Caelo	Potassium citrate	13080603	1
Caelo	Potassium citrate	13135902	1
Caelo	Potassium citrate	13135904	1
Caelo	Potassium citrate	13135907	5
Caelo	Potassium citrate	13135908	1
Caelo	Potassium citrate	1314M-01737	1
Caelo	Potassium citrate	13317602	2
Caelo	Potassium citrate	13317603	2
Caelo	Potassium citrate	13317604	2
Caelo	Potassium citrate	13317613	3
Caelo	Potassium citrate	13317618	2
Caelo	Potassium citrate	14138105	8

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Potassium citrate	14138107	1
Caelo	Potassium citrate	14138112	1
Caelo	Potassium citrate	14138118	3
Caelo	Potassium citrate	14138119	1
Caelo	Potassium citrate	151231	1
Caelo	Potassium citrate	15123102	2
Caelo	Potassium citrate	15123103	4
Caelo	Potassium citrate	15148701	7
Caelo	Potassium citrate	15148702	1
Caelo	Potassium citrate	15148706	11
Caelo	Potassium citrate	15148707	4
Caelo	Potassium citrate	15148708	2
Caelo	Potassium citrate	15158706	1
Caelo	Potassium citrate	15434709	1
Caelo	Potassium citrate	154357	3
Caelo	Potassium citrate	15435701	7
Caelo	Potassium citrate	15435702	1
Caelo	Potassium citrate	154357025	1
Caelo	Potassium citrate	15435703	5
Caelo	Potassium citrate	15435709	3
Caelo	Potassium citrate	15435710	5
Caelo	Potassium citrate	15435711	1
Caelo	Potassium citrate	1543702	1
Caelo	Potassium citrate	15896	1
Caelo	Potassium citrate	16113002	3
Caelo	Potassium citrate	16113003	2
Caelo	Potassium citrate	16113006	6
Caelo	Potassium citrate	16113007	3
Caelo	Potassium citrate	16113008	2
Caelo	Potassium citrate	16113012	10
Caelo	Potassium citrate	17061402	1
Caelo	Potassium citrate	170922904	1
Caelo	Potassium citrate	17092903	8
Caelo	Potassium citrate	17092904	5
Caelo	Potassium citrate	18007603	3
Caelo	Potassium citrate	18007604	2
Caelo	Potassium citrate	18007607	2
Caelo	Potassium citrate	18038502	3
Caelo	Potassium citrate	18038506	11
Caelo	Potassium citrate	18038507	2
Caelo	Potassium citrate	18038509	1
Caelo	Potassium citrate	18038512	2
Caelo	Potassium citrate	18038514	5
Caelo	Potassium citrate	18038517	3
Caelo	Potassium citrate	18038519	4
Caelo	Potassium citrate	18038523	1
Caelo	Potassium citrate	1807034-01	1
Caelo	Potassium citrate	189645	1
Caelo	Potassium citrate	191804001	5
Caelo	Potassium citrate	191804006	6
Caelo	Potassium citrate	191804008	1
Caelo	Potassium citrate	191804009	2
Caelo	Potassium citrate	191804011	1
Caelo	Potassium citrate	19180402	2
Caelo	Potassium citrate	20004139002	2
Caelo	Potassium citrate	20004139003	4
Caelo	Potassium citrate	21000107002	2
Caelo	Potassium citrate	21000107005	1
Caelo	Potassium citrate	21000107010	4
Caelo	Potassium citrate	21000107015	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Potassium citrate	2114M1737	1
Caelo	Potassium citrate	232262310107	1
Caelo	Potassium citrate	26113006	1
Caelo	Potassium citrate	28021402	1
Caelo	Potassium citrate	3012Q-01737	1
Caelo	Potassium citrate	3094247	1
Caelo	Potassium citrate	3112M01737	1
Caelo	Potassium citrate	3456	1
Caelo	Potassium citrate	3618E-01737	1
Caelo	Potassium citrate	411025-1-P	1
Caelo	Potassium citrate	5021509	1
Caelo	Potassium citrate	5555	1
Caelo	Potassium citrate	71730128	2
Caelo	Potassium citrate	71730367	1
Caelo	Potassium citrate	9259107	1
Caelo	Potassium citrate	9259120	1
Caelo	Potassium citrate	Caelo	1
Caelo	Potassium citrate	gfte	1
Caelo	Potassium citrate	RT115113	1
Caesar & Loretz GmbH...	Potassium citrate	19180402	1
Caesar & Loretz GmbH...	Potassium citrate	18038519	1
Caesar & Loretz GmbH...	Potassium citrate	19180402	1
Caesar & Loretz GmbH...	Potassium citrate	191804006	1
Caesar & Loretz GmbH/Gehe	Potassium citrate	191804011	1
Caesar & Loretz GmbH...	Potassium citrate	191804009	1
Caesar & Loretz GmbH...	Potassium citrate	21000107001	1
Caesar & Loretz GmbH...	Potassium citrate	21000107003	1
Caesar & Loretz GmbH/Ph	Potassium citrate	191804006	1
Caesar & Loretz GmbH	Potassium citrate	18007607	1
Caesar & Loretz GmbH	Potassium citrate	18038509	1
Caesar & Loretz GmbH	Potassium citrate	18038514	1
Caesar & Loretz GmbH	Potassium citrate	191804006	1
Caesar & Loretz GmbH	Potassium citrate	191804008	1
Caesar & Loretz GmbH	Potassium citrate	19180401	1
Caesar & Loretz GmbH	Potassium citrate	191804011	1
Caesar & Loretz GmbH	Potassium citrate	19180402	7
Caesar & Loretz GmbH	Potassium citrate	20004139002	1
Caesar & Loretz GmbH	Potassium citrate	20004139003	1
Caesar & Loretz GmbH	Potassium citrate	21000107024	1
EuRho/Phoenix	Potassium citrate	2105012-01	1
EuRho/Phönix	Potassium citrate	1311036-01	1
EuRho	Potassium citrate	1603040-01	1
Eurho	Potassium citrate	2101026-01	1
Euro OT/Phönix	Potassium citrate	3036325	1
Euro OTC	Potassium citrate	1306032-01	1
Euro OTC	Potassium citrate	1311036-01	9
Euro OTC	Potassium citrate	1406025-01	1
Euro OTC	Potassium citrate	1410014-01	2
Euro OTC	Potassium citrate	1504024-01	2
Euro OTC	Potassium citrate	1509044-01	6
Euro OTC	Potassium citrate	1603040-01	12
Euro OTC	Potassium citrate	160601-01	1
Euro OTC	Potassium citrate	160604-01	1
Euro OTC	Potassium citrate	160604101	1
Euro OTC	Potassium citrate	1606041-01	4
Euro OTC	Potassium citrate	1611017	1
Euro OTC	Potassium citrate	1611017-01	8
Euro OTC	Potassium citrate	16113012	1
Euro OTC	Potassium citrate	1705024-01	7
Euro OTC	Potassium citrate	1803003-01	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Potassium citrate	180703401	1
Euro OTC	Potassium citrate	1807034-01	8
Euro OTC	Potassium citrate	1902027	1
Euro OTC	Potassium citrate	1902027-01	7
Euro OTC	Potassium citrate	190227-01	1
Euro OTC	Potassium citrate	190701601	2
Euro OTC	Potassium citrate	1907016-01	2
Euro OTC	Potassium citrate	191200-01	1
Euro OTC	Potassium citrate	1912008-01	9
Euro OTC	Potassium citrate	1912008-02	4
Euro OTC	Potassium citrate	1915A-01737	1
Euro OTC	Potassium citrate	192027-01	1
Euro OTC	Potassium citrate	20004139003	1
Euro OTC	Potassium citrate	2008015-01	7
Euro OTC	Potassium citrate	2008015-02	4
Euro OTC	Potassium citrate	2008015-15	1
Euro OTC	Potassium citrate	2101026-01	6
Euro OTC	Potassium citrate	2105012-01	6
Euro OTC	Potassium citrate	2109025-01	8
Euro OTC	Potassium citrate	2109025-02	2
Euro OTC	Potassium citrate	22101303	1
Euro OTC	Potassium citrate	3126221	1
EuRoh/Noweda	Potassium citrate	1807034-01	1
Fagron	Potassium citrate		1
Fagron	Potassium citrate	123456	6
Fagron	Potassium citrate	1234567	1
Fragon/ Gehe	Potassium citrate	3055187	1
Gatt-Koller	Potassium citrate	1800758	1
Gehe	Potassium citrate	19180402	1
ghfgh	Potassium citrate	3654645	1
Gutenberg-Apotheke	Potassium citrate	13135907	1
Hiperscan	Potassium citrate		1
HiperScan	Potassium citrate		1
L12	Potassium citrate	15435709	1
Labor	Potassium citrate	1234	2
lohmann	Potassium citrate	1051470	1
Nachprüfung	Potassium citrate	111112	1
Nachprüfung	Potassium citrate	123456	1
Noweda 10.12.2019	Potassium citrate	18007607	1
Noweda	Potassium citrate	18038506	1
Noweda	Potassium citrate	21000107014	1
Phoenix 08.07.2014	Potassium citrate	13317624	1
Phoenix Goettin	Potassium citrate	13317613	1
Phoenix	Potassium citrate	1326PLV-1739	1
Phoenix	Potassium citrate	15148708	1
Phönix	Potassium citrate	1211006-01	2
Phönix	Potassium citrate	15123103	1
Sanacorb	Potassium citrate	12135311	2
Sanacorp/ euRho	Potassium citrate	1204016-01	1
Sanacorp	Potassium citrate	14138105	1
Sanacorp	Potassium citrate	160604101	1
Sanacorp	Potassium citrate	191804006	1
Test	Potassium citrate	12345	1
Testsubstanz	Potassium citrate		1

- 235 545 spectra from 1515 *Apo-Ident* customers from a total of 49 094 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Potassium citrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Potassium citrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	550	0	152 412
Type B	0	600	0	201 484
Type C	0	515	7	235 545

The substance/substance group *Potassium citrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9091 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0000 %)
Type C	100.0000 % (> 99.9007 %)	98.6590 % (> 98.0843 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20655	21936	5.41	263.28
21452	22476	8.45	261.47
21775	21936	5.44	263.63
21936	21936	0.00	259.90
22476	22476	0.00	262.76
22921	22921	0.00	258.38
25090	25090	0.00	263.09
25558	25558	0.00	266.30
25607	25607	0.00	257.96
25703	25703	0.00	257.83
26481	26481	0.00	267.73

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**potassium dihydrogen phosphate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10006389-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

potassium dihydrogen phosphate; Kalii dihydrogenophosphas

Special notes

When selecting the *potassium dihydrogen phosphate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
potassium dihydrogen phosphate	3	1	0

Second-stage model

For differentiation of the substance/substance group *potassium dihydrogen phosphate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *potassium dihydrogen phosphate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Silver protein	42.67	–
Carbomers	57.94	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *potassium dihydrogen phosphate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *potassium dihydrogen phosphate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	potassium dihydrogen phosphate	22001752	26567	40	20220615*
Caelo	potassium dihydrogen phosphate	22001752	26567SI	20	20220615*
Caelo	potassium dihydrogen phosphate	23003147	27113	40	20240118*
Caelo	potassium dihydrogen phosphate	23003147	27113SI	20	20240118*
Caelo	potassium dihydrogen phosphate	24002258	27446	40	20241014*
Caelo	potassium dihydrogen phosphate	24002258	27446SI	20	20241014*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 180 spectra of 6 reference samples from the substance/substance group *potassium dihydrogen phosphate*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

- 152 782 spectra from a total of 2839 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *potassium dihydrogen phosphate*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	potassium dihydrogen phosphate	172493	23689	40

- 202 044 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *potassium dihydrogen phosphate*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *potassium dihydrogen phosphate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For

this purpose, all relevant spectra of the various substances were compared with *potassium dihydrogen phosphate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	180	0	152 782
Type B	0	40	0	202 044
Type C	0	0	0	236 067

The substance/substance group *potassium dihydrogen phosphate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26567	26567	0.00	59.48
27113	27113	0.00	56.77
27446	27446	0.00	57.54

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Potassium hydrocarbonate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20193-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Potassium hydrocarbonate; Kalii hydrogencarbonas

Special notes

When selecting the *Potassium hydrocarbonate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Potassium hydrocarbonate	6	2	47

Second-stage model

For differentiation of the substance/substance group *Potassium hydrocarbonate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Potassium hydrocarbonate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	61.33	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Potassium hydrocarbonate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Potassium hydrocarbonate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Potassium hydrocarbonate	23003573	27101	40	20240119*
Euro OTC	Potassium hydrocarbonate	1805027-01	24271	40	20180606
Euro OTC	Potassium hydrocarbonate	2204004	26563	40	20220520*
Euro OTC	Potassium hydrocarbonate	2208022	26564	40	20220902*
Euro OTC	Potassium hydrocarbonate	2208022	26564SI	20	20220902*
Euro OTC	Potassium hydrocarbonate	2303001	26637	40	20230314*
Euro OTC	Potassium hydrocarbonate	2401021	27165	40	20240227*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 260 spectra of 7 reference samples from the substance/substance group *Potassium hydrocarbonate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 702 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 130 spectra of 4 reference samples from the substance/substance group *Potassium hydrocarbonate*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Potassium hydrocarbonate	2107027	25791	50
Euro OTC	Potassium hydrocarbonate	2408009	27454	40
Euro OTC	Potassium hydrocarbonate	2204004	26563SI†	20
Euro OTC	Potassium hydrocarbonate	2303001	26637SI†	20

- 201 954 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 83 spectra from 51 *Apo-Ident* customers from 48 batches from the substance/substance group *Potassium hydrocarbonate*.

- Among them are spectra of independent samples from 47 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Potassium hydrocarbonate	21004124012	1
	Potassium hydrocarbonate	23003573002	1
	Potassium hydrocarbonate	2303001-01	1
	Potassium hydrocarbonate	2401021-01	1
Caelo	Potassium hydrocarbonate		1
Caelo	Potassium hydrocarbonate	10052610	1
Caelo	Potassium hydrocarbonate	10052622	1
Caelo	Potassium hydrocarbonate	10052629	1
Caelo	Potassium hydrocarbonate	1011M-01728	1
Caelo	Potassium hydrocarbonate	11105804	1
Caelo	Potassium hydrocarbonate	11105808	1
Caelo	Potassium hydrocarbonate	11105811	3
Caelo	Potassium hydrocarbonate	11105812	1
Caelo	Potassium hydrocarbonate	11105818	1
Caelo	Potassium hydrocarbonate	11105822	1
Caelo	Potassium hydrocarbonate	1214190	1
Caelo	Potassium hydrocarbonate	12141905	3
Caelo	Potassium hydrocarbonate	12141910	8
Caelo	Potassium hydrocarbonate	12141912	3
Caelo	Potassium hydrocarbonate	12141915	3
Caelo	Potassium hydrocarbonate	12141919	5
Caelo	Potassium hydrocarbonate	12141920	1
Caelo	Potassium hydrocarbonate	12141924	3
Caelo	Potassium hydrocarbonate	12141930	2
Caelo	Potassium hydrocarbonate	1214924	1
Caelo	Potassium hydrocarbonate	12239701	3
Caelo	Potassium hydrocarbonate	12239702	2
Caelo	Potassium hydrocarbonate	12239703	3
Caelo	Potassium hydrocarbonate	1303002-01	1
Caelo	Potassium hydrocarbonate	13141926	1
Caelo	Potassium hydrocarbonate	13390303	1
Caelo	Potassium hydrocarbonate	13390307	1
Caelo	Potassium hydrocarbonate	20080410-3	1
Caelo	Potassium hydrocarbonate	24051301	1
Caelo	Potassium hydrocarbonate	3812Q-01728	1
Caelo	Potassium hydrocarbonate	6011405	1
Caelo	Potassium hydrocarbonate	700544	1
Caelo	Potassium hydrocarbonate	8101202	1
Euro OTC	Potassium hydrocarbonate	1202013-01	1
Euro OTC	Potassium hydrocarbonate	1204038-01	1
Euro OTC	Potassium hydrocarbonate	1208010-01	3
Euro OTC	Potassium hydrocarbonate	1303002-01	3
Euro OTC	Potassium hydrocarbonate	2809033-01	1
Euro OTC	Potassium hydrocarbonate	4413I1728	1
Fagron	Potassium hydrocarbonate	120801001	1
Fagron	Potassium hydrocarbonate	12141911	1
Fagron	Potassium hydrocarbonate	12K27-N06	1
Fagron	Potassium hydrocarbonate	13031205	1
holdermann euro	Potassium hydrocarbonate	1303002-01	1
Noweda	Potassium hydrocarbonate	1004019-01	1
Phoenix	Potassium hydrocarbonate	12141915	1
Stumpf	Potassium hydrocarbonate	1204038-01	1

- 235 984 spectra from 1515 *Apo-Ident* customers from a total of 49 210 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Potassium hydrocarbonate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Potassium hydrocarbonate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	260	0	152 702
Type B	0	130	0	201 954
Type C	0	81	2	235 984

The substance/substance group *Potassium hydrocarbonate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6923 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.3846 %)
Type C	100.0000 % (> 99.9007 %)	97.5904 % (> 93.9759 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24271	27101	9.84	72.13
26563	26563	0.00	73.20
26564	26564	0.00	74.60
26637	26637	0.00	75.07
27101	27101	0.00	73.13
27165	27165	0.00	73.86

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Potassium hydrogen tartrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20509-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Potassium hydrogen tartrate; Kalii hydrogentartras

Special notes

When selecting the *Potassium hydrogen tartrate* substance/substance group, the following information is displayed to the user:

- Advice: Currently no longer available from major pharmaceutical manufacturers. Therefore, batch maintenance is currently not possible.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Potassium hydrogen tartrate	5	3	40

Second-stage model

For differentiation of the substance/substance group *Potassium hydrogen tartrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Potassium hydrogen tartrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Aluminium chloride hexahydrate	86.85	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Potassium hydrogen tartrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Potassium hydrogen tartrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Potassium hydrogen tartrate	11345805	20772	40	20120103
Caelo	Potassium hydrogen tartrate	15354609	23193	40	20151030
Caelo	Potassium hydrogen tartrate	170656	23285	40	20170511*
Caelo	Potassium hydrogen tartrate	182051	24763	40	20180903*
Caelo	Potassium hydrogen tartrate	22001645	26247	40	20220701*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Potassium hydrogen tartrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 762 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Potassium hydrogen tartrate*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Potassium hydrogen tartrate	17065604	23414	40
Caelo	Potassium hydrogen tartrate	17065603	23709	40
Caelo	Potassium hydrogen tartrate	20001056	25288	40
Caelo	Potassium hydrogen tartrate	22001645	26247SI†	20

- 201 944 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 72 spectra from 41 *Apo-Ident* customers from 41 batches from the substance/substance group *Potassium hydrogen tartrate*.

- Among them are spectra of independent samples from 34 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Bären Apotheke	Potassium hydrogen tartrate	15354613	1
Caelo	Potassium hydrogen tartrate	11127417	1
Caelo	Potassium hydrogen tartrate	11345807	1
Caelo	Potassium hydrogen tartrate	13030006	2

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Potassium hydrogen tartrate	13133104	2
Caelo	Potassium hydrogen tartrate	13133114	1
Caelo	Potassium hydrogen tartrate	13133120	2
Caelo	Potassium hydrogen tartrate	13133126	1
Caelo	Potassium hydrogen tartrate	14115208	1
Caelo	Potassium hydrogen tartrate	15081005	1
Caelo	Potassium hydrogen tartrate	15081008	2
Caelo	Potassium hydrogen tartrate	15081010	3
Caelo	Potassium hydrogen tartrate	1534609	1
Caelo	Potassium hydrogen tartrate	15354601	1
Caelo	Potassium hydrogen tartrate	15354604	3
Caelo	Potassium hydrogen tartrate	15354609	3
Caelo	Potassium hydrogen tartrate	15354613	2
Caelo	Potassium hydrogen tartrate	15354614	2
Caelo	Potassium hydrogen tartrate	160514b	1
Caelo	Potassium hydrogen tartrate	17061303	1
Caelo	Potassium hydrogen tartrate	17065603	2
Caelo	Potassium hydrogen tartrate	18205103	2
Caelo	Potassium hydrogen tartrate	18205104	1
Caelo	Potassium hydrogen tartrate	18205106	1
Caelo	Potassium hydrogen tartrate	18205107	1
Caelo	Potassium hydrogen tartrate	20004282003	1
Caelo	Potassium hydrogen tartrate	23062015A	1
Caelo	Potassium hydrogen tartrate	90573259	1
Caesar & Loretz GmbH	Potassium hydrogen tartrate	17366002	1
Caesar & Loretz GmbH	Potassium hydrogen tartrate	182051002	1
Caesar & Loretz GmbH	Potassium hydrogen tartrate	18205101	7
Caesar & Loretz GmbH	Potassium hydrogen tartrate	18205105	1
Caesar & Loretz GmbH	Potassium hydrogen tartrate	18205107	1
Caesar & Loretz GmbH	Potassium hydrogen tartrate	20001056003	1
Caesar & Loretz GmbH	Potassium hydrogen tartrate	20001056005	1
Caleo/ Noweda	Potassium hydrogen tartrate	18205103	1
Gehe	Potassium hydrogen tartrate	11345808	1
Hänseler	Potassium hydrogen tartrate		6
Lamotte/Phönix	Potassium hydrogen tartrate	17065602	1
phönix	Potassium hydrogen tartrate	15354604	1
Phönix	Potassium hydrogen tartrate	20004282003	1
Sanacorp	Potassium hydrogen tartrate	14115208	3
Sanacorp	Potassium hydrogen tartrate	15354609	1
Sanacorp	Potassium hydrogen tartrate	20001056003	1
Sanacorp	Potassium hydrogen tartrate	20001056005	1

- 235 995 spectra from 1515 *Apo-Ident* customers from a total of 49 217 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Potassium hydrogen tartrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Potassium hydrogen tartrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	140	0	201 944
Type C	0	71	1	235 995

The substance/substance group *Potassium hydrogen tartrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	98.6111 % (> 94.4444 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20772	23285	9.17	176.58
23193	23285	5.79	178.69
23285	23285	0.00	174.28
24763	24763	0.00	175.22
26247	26247	0.00	176.90

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Potassium sorbate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20020-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Potassium sorbate; Kalii sorbas

Special notes

When selecting the *Potassium sorbate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Potassium sorbate	9	12	223

Second-stage model

For differentiation of the substance/substance group *Potassium sorbate* the following second-stage model is used:

- Submodel 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Potassium sorbate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	124.15	–
⋮	⋮	⋮
Mometasone furoate	>50	37.68
Atropine sulfate	>50	101.29
Hydrocortisone	>50	159.33
Magnesium hydrogen citrate	>50	180.42
Propranolol hydrochloride	>50	281.87
Quinoline yellow	>50	383.81
Escin, water-soluble	>50	425.63
Phenytoin	>50	495.57
Saccharin sodium	>50	584.30
Calcium orotate dihydrate	>50	668.21

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Potassium sorbate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Potassium sorbate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Potassium sorbate	13224604	21444	60	20130813
Caelo	Potassium sorbate	163266	23059	40	20170105*
Caelo	Potassium sorbate	17170008	23585	30	20170711
Caelo	Potassium sorbate	20001879	25556	40	20200714*
Caelo	Potassium sorbate	20001880	25630	40	20200714*
Caelo	Potassium sorbate	23001012	26713	40	20230516*
Caelo	Potassium sorbate	23001012	26713SI	20	20230516*
Euro OTC	Potassium sorbate	1508025	21892	60	20150902*
Euro OTC	Potassium sorbate	1608013	22786	40	20160819*
Euro OTC	Potassium sorbate	1907023	24764	40	20190802*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 410 spectra of 10 reference samples from the substance/substance group *Potassium sorbate*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 552 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 530 spectra of 14 reference samples from the substance/substance group *Potassium sorbate*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Potassium sorbate	171700	23638	40
Caelo	Potassium sorbate	173451	23830	40
Caelo	Potassium sorbate	181650	24224	40
Caelo	Potassium sorbate	191072	24539	40
Caelo	Potassium sorbate	21001391	25700	50
Caelo	Potassium sorbate	22002065	26244	40
Caelo	Potassium sorbate	23002441	26944	40
Caelo	Potassium sorbate	23002442	26961	40
Euro OTC	Potassium sorbate	1703034	23176	40
Euro OTC	Potassium sorbate	1710015	23772	40
Euro OTC	Potassium sorbate	1805029	24126	40
Euro OTC	Potassium sorbate	1901020	24464	40
Caelo	Potassium sorbate	22002065	26244SI	20
Caelo	Potassium sorbate	23002441	26944SI	20

- 201 554 spectra from a total of 4033 batches from further 838 substances. These spectra were

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1921 spectra from 981 *Apo-Ident* customers from 228 batches from the substance/substance group *Potassium sorbate*.
- Among them are spectra of independent samples from 223 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Potassium sorbate		1
	Potassium sorbate	10012203	1
	Potassium sorbate	12211101	2
	Potassium sorbate	17170017	1
	Potassium sorbate	19000555010	1
	Potassium sorbate	20004207005	1
	Potassium sorbate	20004356001	1
	Potassium sorbate	22002065002	1
	Potassium sorbate	22003409002	1
	Potassium sorbate	22003409004	2
	Potassium sorbate	22003409007	12
	Potassium sorbate	22003409010	2
	Potassium sorbate	22003409013	9
	Potassium sorbate	22003409014	8
	Potassium sorbate	23001012004	18
	Potassium sorbate	23001012010	1
	Potassium sorbate	922331021	1
/Alliance	Potassium sorbate	18165010	1
AHD	Potassium sorbate	13065216	1
AHD	Potassium sorbate	17170007	1
AHD	Potassium sorbate	17345116	1
AHD	Potassium sorbate	216331021	1
AHD	Potassium sorbate	22003409004	1
AHD	Potassium sorbate	22003409013	1
AHD	Potassium sorbate	23001012004	1
Alliance Healthcare	Potassium sorbate	15382115	1
Alliance Healthcare	Potassium sorbate	20004207002	1
Allianz	Potassium sorbate	17170006	1
Anzag 12.01.15	Potassium sorbate	13224611	1
Anzag	Potassium sorbate	12211107	1
Anzag	Potassium sorbate	15382114	2
Anzag	Potassium sorbate	20004207005	1
Anzag	Potassium sorbate	23001012004	1
apomix	Potassium sorbate	13224611	1
apomix	Potassium sorbate	17345104	1
Bombastus	Potassium sorbate	1117331022	1
Bombastus	Potassium sorbate	14380632	1
Caeleo/ Kehr	Potassium sorbate	20004207002	1
Caelo	Potassium sorbate		2
Caelo	Potassium sorbate	1/1/0017	1
Caelo	Potassium sorbate	10012210	1
Caelo	Potassium sorbate	10199505	1
Caelo	Potassium sorbate	111033102	1
Caelo	Potassium sorbate	1112331024	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Potassium sorbate	1118331022	1
Caelo	Potassium sorbate	11192305	3
Caelo	Potassium sorbate	11214207	1
Caelo	Potassium sorbate	11261304	3
Caelo	Potassium sorbate	12059902	1
Caelo	Potassium sorbate	12059905	2
Caelo	Potassium sorbate	12059908	2
Caelo	Potassium sorbate	12059909	4
Caelo	Potassium sorbate	12059914	2
Caelo	Potassium sorbate	1205999	1
Caelo	Potassium sorbate	12211101	10
Caelo	Potassium sorbate	12211102	4
Caelo	Potassium sorbate	12211107	16
Caelo	Potassium sorbate	12211108	2
Caelo	Potassium sorbate	12211121	4
Caelo	Potassium sorbate	12211123	1
Caelo	Potassium sorbate	12345	1
Caelo	Potassium sorbate	13065204	11
Caelo	Potassium sorbate	13065205	12
Caelo	Potassium sorbate	13065211	1
Caelo	Potassium sorbate	13065216	11
Caelo	Potassium sorbate	13065217	11
Caelo	Potassium sorbate	13065222	1
Caelo	Potassium sorbate	13111409	1
Caelo	Potassium sorbate	1312024-01	2
Caelo	Potassium sorbate	13224604	17
Caelo	Potassium sorbate	13224608	2
Caelo	Potassium sorbate	13224610	1
Caelo	Potassium sorbate	13224611	12
Caelo	Potassium sorbate	13224612	18
Caelo	Potassium sorbate	13277804	1
Caelo	Potassium sorbate	1397235	1
Caelo	Potassium sorbate	14140007	1
Caelo	Potassium sorbate	14192605	2
Caelo	Potassium sorbate	143806	1
Caelo	Potassium sorbate	1438060	2
Caelo	Potassium sorbate	14380601	18
Caelo	Potassium sorbate	14380602	2
Caelo	Potassium sorbate	14380606	9
Caelo	Potassium sorbate	14380607	10
Caelo	Potassium sorbate	14380610	13
Caelo	Potassium sorbate	14380612	2
Caelo	Potassium sorbate	14380613	1
Caelo	Potassium sorbate	14380618	1
Caelo	Potassium sorbate	14380620	6
Caelo	Potassium sorbate	14380621	11
Caelo	Potassium sorbate	14380622	12
Caelo	Potassium sorbate	14380627	10
Caelo	Potassium sorbate	14380631	1
Caelo	Potassium sorbate	14380632	23
Caelo	Potassium sorbate	14380633	16
Caelo	Potassium sorbate	14380635	8
Caelo	Potassium sorbate	14382606	1
Caelo	Potassium sorbate	1438633	1
Caelo	Potassium sorbate	1508025-01	1
Caelo	Potassium sorbate	15248203	3
Caelo	Potassium sorbate	15248204	20
Caelo	Potassium sorbate	15248205	11
Caelo	Potassium sorbate	15382103	1
Caelo	Potassium sorbate	15382105	16

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Potassium sorbate	15382106	1
Caelo	Potassium sorbate	15382114	13
Caelo	Potassium sorbate	15382115	11
Caelo	Potassium sorbate	1608013-01	1
Caelo	Potassium sorbate	16156505	4
Caelo	Potassium sorbate	16326602	4
Caelo	Potassium sorbate	16326606	20
Caelo	Potassium sorbate	16326607	17
Caelo	Potassium sorbate	16326608	21
Caelo	Potassium sorbate	16326609	20
Caelo	Potassium sorbate	16326615	1
Caelo	Potassium sorbate	17170002	4
Caelo	Potassium sorbate	17170005	1
Caelo	Potassium sorbate	17170006	13
Caelo	Potassium sorbate	17170007	26
Caelo	Potassium sorbate	17170007-20171106Ma1	1
Caelo	Potassium sorbate	17170008	25
Caelo	Potassium sorbate	17170012	5
Caelo	Potassium sorbate	17170013	32
Caelo	Potassium sorbate	17170014	34
Caelo	Potassium sorbate	17170015	2
Caelo	Potassium sorbate	17170016	3
Caelo	Potassium sorbate	17170016P-190225-3	1
Caelo	Potassium sorbate	17170017	19
Caelo	Potassium sorbate	17170018	1
Caelo	Potassium sorbate	1717008	1
Caelo	Potassium sorbate	17345103	33
Caelo	Potassium sorbate	17345104	58
Caelo	Potassium sorbate	17345105	1
Caelo	Potassium sorbate	17345113	3
Caelo	Potassium sorbate	17345116	36
Caelo	Potassium sorbate	18(19000555006)	1
Caelo	Potassium sorbate	18165006	32
Caelo	Potassium sorbate	18165010	56
Caelo	Potassium sorbate	18165014	25
Caelo	Potassium sorbate	18165015	31
Caelo	Potassium sorbate	18165016	2
Caelo	Potassium sorbate	18165016P-190923-1	1
Caelo	Potassium sorbate	1816510	1
Caelo	Potassium sorbate	190000555006	1
Caelo	Potassium sorbate	190000555010	1
Caelo	Potassium sorbate	190000555011	2
Caelo	Potassium sorbate	1900055006	2
Caelo	Potassium sorbate	1900055011	4
Caelo	Potassium sorbate	19000555005	4
Caelo	Potassium sorbate	19000555006	59
Caelo	Potassium sorbate	190005550066	1
Caelo	Potassium sorbate	19000555009	1
Caelo	Potassium sorbate	19000555010	37
Caelo	Potassium sorbate	19000555011	37
Caelo	Potassium sorbate	1900055505	2
Caelo	Potassium sorbate	1900055506	3
Caelo	Potassium sorbate	1900055510	1
Caelo	Potassium sorbate	1900555010	1
Caelo	Potassium sorbate	191072008	1
Caelo	Potassium sorbate	19107203	3
Caelo	Potassium sorbate	19107203P-200518-1	1
Caelo	Potassium sorbate	19107206	1
Caelo	Potassium sorbate	19107207	2
Caelo	Potassium sorbate	19107208	41

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Potassium sorbate	19107280	1
Caelo	Potassium sorbate	198000555006	1
Caelo	Potassium sorbate	200004207002	1
Caelo	Potassium sorbate	200004207005	1
Caelo	Potassium sorbate	200004356006	1
Caelo	Potassium sorbate	20004207002	42
Caelo	Potassium sorbate	20004207005	45
Caelo	Potassium sorbate	20004356001	36
Caelo	Potassium sorbate	20004356011	14
Caelo	Potassium sorbate	2000435611	1
Caelo	Potassium sorbate	20021112-2	1
Caelo	Potassium sorbate	2004207002	1
Caelo	Potassium sorbate	2004207005	3
Caelo	Potassium sorbate	2004356001	1
Caelo	Potassium sorbate	200613K1	1
Caelo	Potassium sorbate	20082001	1
Caelo	Potassium sorbate	2041402	1
Caelo	Potassium sorbate	21001391008	2
Caelo	Potassium sorbate	22002065002	11
Caelo	Potassium sorbate	22003409001	1
Caelo	Potassium sorbate	22003409002	2
Caelo	Potassium sorbate	22003409003	2
Caelo	Potassium sorbate	22003409004	14
Caelo	Potassium sorbate	22003409007	12
Caelo	Potassium sorbate	22003409013	2
Caelo	Potassium sorbate	22003409014	1
Caelo	Potassium sorbate	220905(22002065002)	1
Caelo	Potassium sorbate	23001012004	1
Caelo	Potassium sorbate	27101705	1
Caelo	Potassium sorbate	317331021	2
Caelo	Potassium sorbate	3354	1
Caelo	Potassium sorbate	3512M-01748	1
Caelo	Potassium sorbate	7111805	1
Caelo	Potassium sorbate	8165015	1
Caelo	Potassium sorbate	90318101	1
Caelo	Potassium sorbate	9061806	1
Caelo	Potassium sorbate	912331023	1
Caelo	Potassium sorbate	91623299	2
Caelo	Potassium sorbate	9305601	2
Caelo	Potassium sorbate	AKD10	1
Caelo	Potassium sorbate	K-010213-1	1
Caelo	Potassium sorbate	RT287	1
Caelo	Potassium sorbate	RT5324	1
Caesar & Lorenz GmbH	Potassium sorbate	19000555006	1
Caesar & Lorenz/Noweda	Potassium sorbate	20004356001	1
Caesar & Loretz GmbH...	Potassium sorbate	171700006	1
Caesar & Loretz GmbH...	Potassium sorbate	19107208	2
Caesar & Loretz GmbH...	Potassium sorbate	15382114	1
Caesar & Loretz GmbH...	Potassium sorbate	17345103	1
Caesar & Loretz GmbH...	Potassium sorbate	18165015	1
Caesar & Loretz GmbH...	Potassium sorbate	20004207005	1
Caesar & Loretz GmbH...	Potassium sorbate	20004356011	1
Caesar & Loretz GmbH...	Potassium sorbate	20004207005	1
Caesar & Loretz GmbH...	Potassium sorbate	13065217	2
Caesar & Loretz GmbH...	Potassium sorbate	19000555010	1
Caesar & Loretz GmbH...	Potassium sorbate	20004356011	1
Caesar & Loretz GmbH...	Potassium sorbate	22003409004	1
Caesar & Loretz GmbH...	Potassium sorbate	19000555010	1
Caesar & Loretz GmbH...	Potassium sorbate	17170017	1
Caesar & Loretz GmbH/AHD	Potassium sorbate	19107203	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH…	Potassium sorbate	19000555010	1
Caesar & Loretz GmbH…	Potassium sorbate	18165015	1
Caesar & Loretz GmbH…	Potassium sorbate	20004207002	1
Caesar & Loretz GmbH…	Potassium sorbate	1900055510	1
Caesar & Loretz GmbH/Gehe	Potassium sorbate	18165014	1
Caesar & Loretz GmbH/Gehe	Potassium sorbate	190000555006	1
Caesar & Loretz GmbH/Gehe	Potassium sorbate	19000555006	1
Caesar & Loretz GmbH/Gehe	Potassium sorbate	20004207002	1
Caesar & Loretz GmbH/Gehe	Potassium sorbate	20004207005	2
Caesar & Loretz GmbH/Gehe	Potassium sorbate	22003409014	1
Caesar & Loretz GmbH…	Potassium sorbate	20004207002	1
Caesar & Loretz GmbH/K	Potassium sorbate	19107208	1
Caesar & Loretz GmbH/Kehr	Potassium sorbate	19000555010	1
Caesar & Loretz GmbH…	Potassium sorbate	19107208	1
Caesar & Loretz GmbH/Now	Potassium sorbate	20004207005	1
Caesar & Loretz GmbH…	Potassium sorbate	19000555006	2
Caesar & Loretz GmbH…	Potassium sorbate	20004207002	1
Caesar & Loretz GmbH…	Potassium sorbate	20004356011	1
Caesar & Loretz GmbH…	Potassium sorbate	19000555011	1
Caesar & Loretz GmbH…	Potassium sorbate	20004207002	1
Caesar & Loretz GmbH…	Potassium sorbate	20004356001	1
Caesar & Loretz GmbH…	Potassium sorbate	22003409003	1
Caesar & Loretz GmbH…	Potassium sorbate	17345104	1
Caesar & Loretz GmbH…	Potassium sorbate	18165014	1
Caesar & Loretz GmbH…	Potassium sorbate	19000555008	1
Caesar & Loretz GmbH…	Potassium sorbate	19107208	2
Caesar & Loretz GmbH…	Potassium sorbate	20004207002	1
Caesar & Loretz GmbH…	Potassium sorbate	22003409002	1
Caesar & Loretz GmbH	Potassium sorbate	11261303	1
Caesar & Loretz GmbH	Potassium sorbate	14380627	1
Caesar & Loretz GmbH	Potassium sorbate	17170006	1
Caesar & Loretz GmbH	Potassium sorbate	17345103	1
Caesar & Loretz GmbH’	Potassium sorbate	17345109	2
Caesar & Loretz GmbH	Potassium sorbate	18165002	1
Caesar & Loretz GmbH	Potassium sorbate	18165004	1
Caesar & Loretz GmbH	Potassium sorbate	18165006	1
Caesar & Loretz GmbH	Potassium sorbate	18165010	12
Caesar & Loretz GmbH	Potassium sorbate	18165014	4
Caesar & Loretz GmbH	Potassium sorbate	18165015	6
Caesar & Loretz GmbH	Potassium sorbate	19000555005	3
Caesar & Loretz GmbH	Potassium sorbate	19000555006	17
Caesar & Loretz GmbH	Potassium sorbate	19000555008	3
Caesar & Loretz GmbH	Potassium sorbate	19000555009	3
Caesar & Loretz GmbH	Potassium sorbate	19000555010	10
Caesar & Loretz GmbH	Potassium sorbate	19000555011	6
Caesar & Loretz GmbH	Potassium sorbate	19107203	1
Caesar & Loretz GmbH	Potassium sorbate	19107208	15
Caesar & Loretz GmbH	Potassium sorbate	20001879002	2
Caesar & Loretz GmbH	Potassium sorbate	20004207002	24
Caesar & Loretz GmbH	Potassium sorbate	20004207005	11
Caesar & Loretz GmbH	Potassium sorbate	20004207006	2
Caesar & Loretz GmbH	Potassium sorbate	20004356001	15
Caesar & Loretz GmbH	Potassium sorbate	20004356003	2
Caesar & Loretz GmbH	Potassium sorbate	20004356011	4
Caesar & Loretz GmbH	Potassium sorbate	20004498001	1
Caesar & Loretz GmbH	Potassium sorbate	22002065002	5
Caesar & Loretz GmbH	Potassium sorbate	22002065003	1
Caesar & Loretz GmbH	Potassium sorbate	22003409002	5
Caesar & Loretz GmbH	Potassium sorbate	22003409004	3
Caesar & Loretz GmbH	Potassium sorbate	22003409007	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Potassium sorbate	22003409013	1
Caesar & Loretz GmbH...	Potassium sorbate	19000555011	1
Caesar & Loretz GmbH...	Potassium sorbate	22002065002	1
Caesar & Loretz/Geil...	Potassium sorbate	19000555006	1
Caesar & Loretz/Noweda	Potassium sorbate	14380621	1
Caesar & Loretz/Noweda	Potassium sorbate	19000555010	1
Caesar & Loretz/Sanacorp	Potassium sorbate	17345104	1
Caesar & Loretz	Potassium sorbate	14380606	2
Caesar & Loretz	Potassium sorbate	14380633	1
Caesar & Loretz	Potassium sorbate	17345103	1
Caesar & Loretz	Potassium sorbate	19000555010	1
Caesar / Gehe	Potassium sorbate	14380622	1
Caesar und Loretz	Potassium sorbate	18165010	1
Caesar&Loretz GmbH/S...	Potassium sorbate	14380607	1
Caesar&Loretz GmbH	Potassium sorbate	14380622	1
Caesar&Loretz GmbH	Potassium sorbate	17170014	1
Caesar/Gehe	Potassium sorbate	19107208	1
Caesar/Lorenz	Potassium sorbate	13065204	1
Caleo/Krieger	Potassium sorbate	20004356001	1
canea, gehe	Potassium sorbate	13065215	1
Cealo/ Noweda	Potassium sorbate	17345103	1
cealo	Potassium sorbate	16326607	1
Cealo	Potassium sorbate	16326609	1
Cealo	Potassium sorbate	1710013	1
Euro OTC	Potassium sorbate	1111038-01	1
Euro OTC	Potassium sorbate	111103802	1
Euro OTC	Potassium sorbate	1111038-02	2
Euro OTC	Potassium sorbate	1312024-01	3
Euro OTC	Potassium sorbate	13224612	1
Euro OTC	Potassium sorbate	14380622	1
Euro OTC	Potassium sorbate	14380632	2
Euro OTC	Potassium sorbate	1508025-01	7
Euro OTC	Potassium sorbate	15382115	1
Euro OTC	Potassium sorbate	1608013-01	8
Euro OTC	Potassium sorbate	1710012-01	1
Euro OTC	Potassium sorbate	1710015-01	1
Euro OTC	Potassium sorbate	17170008	1
Euro OTC	Potassium sorbate	17170013	1
Euro OTC	Potassium sorbate	1805029-01	1
Euro OTC	Potassium sorbate	180529-01	1
Euro OTC	Potassium sorbate	1901020-01	5
Euro OTC	Potassium sorbate	1907023-01	1
Euro OTC	Potassium sorbate	1907023-02	1
Euro OTC	Potassium sorbate	1991020-01	1
Euro OTC	Potassium sorbate	216331021	1
Euro OTC	Potassium sorbate	PS20180905	1
Fagron	Potassium sorbate	1114331022	1
Fagron	Potassium sorbate	13065217	1
Fagron	Potassium sorbate	14380622	1
Fagron	Potassium sorbate	16326609	1
Fagron	Potassium sorbate	17170008	1
Fagron	Potassium sorbate	17170013	2
Fagron	Potassium sorbate	17170014	1
Fagron	Potassium sorbate	2717M-01748	1
Fagron	Potassium sorbate	3115M-01748	1
Fagron	Potassium sorbate	3518A-01748	1
Fagron	Potassium sorbate	3912A-01748	1
Fagron	Potassium sorbate	4314U-01748	1
Fresenius	Potassium sorbate	220214221	1
Gehe / Spinnrad	Potassium sorbate	216331021	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Potassium sorbate	11261304	1
Gehe	Potassium sorbate	123331021	1
Gehe	Potassium sorbate	13065205	1
Gehe	Potassium sorbate	13065216	1
Gehe	Potassium sorbate	14380601	1
Gehe	Potassium sorbate	14380607	1
Gehe	Potassium sorbate	14380632	1
Gehe	Potassium sorbate	16326606	1
Gehe	Potassium sorbate	17170007	2
GEHE	Potassium sorbate	17170008	1
Gehe	Potassium sorbate	17170013	1
gehe	Potassium sorbate	17170014	1
Gehe	Potassium sorbate	17345116	1
Gehe	Potassium sorbate	18165010	1
Gehe	Potassium sorbate	18165014	1
Gehe	Potassium sorbate	19000555006	1
Gehe	Potassium sorbate	200004207005	1
Gehe	Potassium sorbate	20004207005	1
Gehe	Potassium sorbate	22003409004	1
Gehe	Potassium sorbate	22003409007	1
GEHE	Potassium sorbate	22003409007	1
Gehe	Potassium sorbate	23001012004	1
Geibo	Potassium sorbate	17170013	1
Ichthyol/Noweda	Potassium sorbate	13224604	1
Ichthyol-Gesellschaf...	Potassium sorbate	18165014	1
Jenne	Potassium sorbate	17170007	1
Jenne	Potassium sorbate	22003409013	1
jenne	Potassium sorbate	922331021	1
Kehr/Spinnrad	Potassium sorbate	317331021	1
Kehr	Potassium sorbate	16326607	1
Kehr	Potassium sorbate	18165006	1
Kehr	Potassium sorbate	22003409013	1
Kehr	Potassium sorbate	23001012004	1
Noweda / Spinnrad	Potassium sorbate	216331021	1
Noweda/ Spinnrad	Potassium sorbate	218331021	1
Noweda/Caesar & Lore...	Potassium sorbate	22003409004	1
Noweda/Spinnrad GmbH	Potassium sorbate	322331021	1
Noweda/Spinnrad	Potassium sorbate	19170208	1
Noweda	Potassium sorbate	12211101	1
Noweda	Potassium sorbate	13065222	1
Noweda	Potassium sorbate	15382115	1
Noweda	Potassium sorbate	16326606	1
Noweda	Potassium sorbate	17170014	1
Noweda	Potassium sorbate	17170017	1
Noweda	Potassium sorbate	17345103	1
Noweda	Potassium sorbate	17345116	1
Noweda	Potassium sorbate	18165010	4
Noweda	Potassium sorbate	20004207005	3
Noweda	Potassium sorbate	22003409014	1
Noweda	Potassium sorbate	23001012004	3
p&m cosmetics/gehe	Potassium sorbate	17170014	1
Phoenix	Potassium sorbate	1117331022	1
Phoenix	Potassium sorbate	1397235	1
Phoenix	Potassium sorbate	14380627	1
Phoenix	Potassium sorbate	17170012	1
Phoenix	Potassium sorbate	17170017	1
Phoenix	Potassium sorbate	17345104	1
Phoenix	Potassium sorbate	20004207002	1
Phoenix	Potassium sorbate	20004207005	1
Phoenix	Potassium sorbate	216331021	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Potassium sorbate	22002065002	1
Phönix/Spinnrad	Potassium sorbate	1117331022	2
phönix	Potassium sorbate	14380632	1
Phönix	Potassium sorbate	16326607	1
phönix	Potassium sorbate	16326608	1
Phönix	Potassium sorbate	17345116	1
PHÖNIX	Potassium sorbate	19000555006	1
Phönix	Potassium sorbate	19000555011	1
Phönix	Potassium sorbate	20004207002	1
Phönix	Potassium sorbate	201103010	1
Phönix	Potassium sorbate	22003409014	1
s.Prüfprotokoll	Potassium sorbate		1
sana	Potassium sorbate	13224612	1
Sanacorp 29.10.18 EK 4,30	Potassium sorbate	17345104	1
Sanacorp	Potassium sorbate	1118331022	1
Sanacorp	Potassium sorbate	12211101	1
Sanacorp	Potassium sorbate	13065217	1
Sanacorp	Potassium sorbate	13224611	1
Sanacorp	Potassium sorbate	14380610	1
Sanacorp	Potassium sorbate	17170007	1
Sanacorp	Potassium sorbate	17170014	1
Sanacorp	Potassium sorbate	19107208	3
Sanacorp	Potassium sorbate	20004207005	1
Sanacorp	Potassium sorbate	22003409014	1
Sanacorp	Potassium sorbate	23001012004	3
sanacorp	Potassium sorbate	2300102004	1
Sanacorp	Potassium sorbate	322331021	1
siehe WE-Prüfprotokoll	Potassium sorbate	61/11	1
Sonnenberg-Apotheke	Potassium sorbate	13224604	1
Spinnrad - Noweda	Potassium sorbate	315331021	1
Spinnrad / Gehe	Potassium sorbate	317331021	2
Spinnrad / Gehe	Potassium sorbate	616331022	1
Spinnrad GmbH / Nowe...	Potassium sorbate	1117331022	1
Spinnrad GmbH Bad Se...	Potassium sorbate	1019331022	1
Spinnrad GmbH Bad Se...	Potassium sorbate	1118331022	1
Spinnrad GmbH	Potassium sorbate	111033102	1
Spinnrad GmbH	Potassium sorbate	1114331022	1
Spinnrad GmbH	Potassium sorbate	214331021	1
spinnrad GmbH	Potassium sorbate	616331022	1
Spinnrad GmbH	Potassium sorbate	912331023	2
Spinnrad Noweda	Potassium sorbate	520331021	1
Spinnrad Noweda	Potassium sorbate	7203311027	1
Spinnrad/ Gehe 18.01.19	Potassium sorbate	317331021	1
Spinnrad/ Noweda/ 26...	Potassium sorbate	319331021	1
Spinnrad/ Phönix	Potassium sorbate	322331021	1
spinnrad/gehe	Potassium sorbate	216331021	1
Spinnrad/Gehe	Potassium sorbate	315331021	1
spinnrad/Noweda	Potassium sorbate	1019331022	1
Spinnrad/Noweda	Potassium sorbate	1117331022	2
Spinnrad/Noweda	Potassium sorbate	1118331022	2
Spinnrad/Noweda	Potassium sorbate	218331021	1
Spinnrad/Noweda	Potassium sorbate	520331021	1
Spinnrad/Noweda	Potassium sorbate	720331022	1
Spinnrad/Noweda	Potassium sorbate	922331021	1
Spinnrad/Phoenix	Potassium sorbate	1019331022	1
Spinnrad/Phoenix	Potassium sorbate	317331021	1
Spinnrad/Phönix	Potassium sorbate	1019331022	1
Spinnrad/Phönix	Potassium sorbate	1118331022	1
Spinnrad/Phönix	Potassium sorbate	218331021	1
Spinnrad/Phönix	Potassium sorbate	319331021	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Spinnrad/Sannacorp	Potassium sorbate	616331022	1
Spinnrad	Potassium sorbate	111033102	1
spinnrad	Potassium sorbate	1114331022	1
Spinnrad	Potassium sorbate	1114331022	3
spinnrad	Potassium sorbate	1117331022	1
Spinnrad	Potassium sorbate	1117331022	2
spinnrad	Potassium sorbate	1118331022	1
Spinnrad	Potassium sorbate	1118331022	1
Spinnrad	Potassium sorbate	214331021	1
spinnrad	Potassium sorbate	216331021	1
Spinnrad	Potassium sorbate	216331021	2
spinnrad	Potassium sorbate	2233102	1
Spinnrad	Potassium sorbate	312331021	2
Spinnrad	Potassium sorbate	315331021	2
spinnrad	Potassium sorbate	317331021	1
Spinnrad	Potassium sorbate	317331021	3
spinnrad	Potassium sorbate	520331021	1
Spinnrad	Potassium sorbate	520331021	3
spinnrad	Potassium sorbate	616331022	1
Spinnrad	Potassium sorbate	616331022	2
spinnrad	Potassium sorbate	720331022	2
Spinnrad	Potassium sorbate	720331022	1
Spinnrad	Potassium sorbate	815331022	2
Spinnrad	Potassium sorbate	912331023	4
Spinrad/Phönix	Potassium sorbate	218331021	1
WE: über Eyach 5g/2,…	Potassium sorbate	14380601	1
wie gehbat	Potassium sorbate	wiegehabt	1

- 234 146 spectra from 1515 *Apo-Ident* customers from a total of 49 034 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Potassium sorbate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Potassium sorbate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	410	0	152 552
Type B	0	530	0	201 554
Type C	0	1919	2	234 146

The substance/substance group *Potassium sorbate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5366 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8679 %)
Type C	100.0000 % (> 99.9007 %)	99.8959 % (> 99.7397 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21444	21892	15.19	200.11
21892	21892	0.00	198.68
22786	22786	0.00	196.67
23059	23059	0.00	207.15
23585	25630	19.20	205.30
24764	24764	0.00	197.95
25556	25556	0.00	204.01
25630	25630	0.00	204.51
26713	26713	0.00	203.18

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Povidone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20684-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Povidone; Povidonum

Special notes

When selecting the *Povidone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Povidone	15	8	57

Second-stage model

For differentiation of the substance/substance group *Povidone* the following second-stage model is used:

- Submodel 05

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Povidone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Povidone iodine	27.69	11.08
Progesterone	69.45	54.06
⋮	⋮	⋮
Spironolactone	>50	46.09
Fusidic acid	85.20	50.44
Testosterone propionate	>50	73.01
Ubidecarenone	>50	126.19

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Povidone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Povidone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Povidone	12032714	20684	40	1402437
Caelo	Povidone	14142103	21378	40	AR-15-FG-000596-01
Caelo	Povidone	16307808	23255	40	AR-17-FG-015299-02
Caelo	Povidone	180276	24044	40	20180202*
Caelo	Povidone	191752	24746	40	20190717*
Caelo	Povidone	191276	24754	40	20190517*
Caelo	Povidone	20000212	25194	40	20200313*
Caelo	Povidone	20003415	25624	40	20201116*
Caelo	Povidone	21003749	26003	40	20220203*
Caelo	Povidone	23001270	26831	40	20230627*
Caelo	Povidone	24000976	27335	40	20240826*
Fagron	Povidone	12E22-N05	20770	40	1411537
Fagron	Povidone	13J21-N02	22731	40	AR-16-FG-019116-01
Fagron	Povidone	15C12-B02-323006	23265	40	1710348
Fagron	Povidone	21I30-B03-219629	26287	40	20220510

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 600 spectra of 15 reference samples from the substance/substance group *Povidone*. These samples are listed above in the *calibration samples* section. The reference samples come from 15 different batches.

- 152 362 spectra from a total of 2827 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 380 spectra of 11 reference samples from the substance/substance group *Povidone*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Povidone	172091	23619	40
Caelo	Povidone	180766	24245	40
Caelo	Povidone	181820	24246	40
Caelo	Povidone	182383	24291	40
Caelo	Povidone	183000	24396	40
Caelo	Povidone	192500	24899	40
Caelo	Povidone	23002064	26953	40
Fagron	Povidone	23E05-B03-228683	26917	40
Caelo	Povidone	21003749	26003SI†	20
Caelo	Povidone	23001270	26831SI†	20
Fagron	Povidone	21I30-B03-219629	26287SI†	20

- 201 704 spectra from a total of 4034 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 184 spectra from 72 *Apo-Ident* customers from 60 batches from the substance/substance group *Povidone*.
- Among them are spectra of independent samples from 57 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Povidone	23001270003	1
21001192005	Povidone	21001192005	1
Alliance	Povidone	16307808	1
Alliance	Povidone	17209106	1
Alliance	Povidone	18112201	1
Audor Pharma	Povidone	18112201	1
Caelo	Povidone	12032714	1
Caelo	Povidone	12376301	1
Caelo	Povidone	13323407	2
Caelo	Povidone	14142103	1
Caelo	Povidone	14142109	3
Caelo	Povidone	14207508	3
Caelo	Povidone	14207511	4
Caelo	Povidone	14207515	1
Caelo	Povidone	14207517	1
Caelo	Povidone	15013721	1
Caelo	Povidone	15383101	3
Caelo	Povidone	15383102	1
Caelo	Povidone	15383103	2
Caelo	Povidone	16051101	2
Caelo	Povidone	16051102	1
Caelo	Povidone	16051103	1
Caelo	Povidone	16051104	1
Caelo	Povidone	16051108	2
Caelo	Povidone	16051110	1
Caelo	Povidone	16307802	1
Caelo	Povidone	16307808	1
Caelo	Povidone	163078085328	1
Caelo	Povidone	16307809	5
Caelo	Povidone	16307811	3
Caelo	Povidone	16307812	1
Caelo	Povidone	17209103	2
Caelo	Povidone	17209104	3
Caelo	Povidone	17209110	1
Caelo	Povidone	18024602	1
Caelo	Povidone	18027602	5
Caelo	Povidone	18112201	4
Caelo	Povidone	18182002	2
Caelo	Povidone	18238302	1
Caelo	Povidone	18300002	3
Caelo	Povidone	18300003	1
Caelo	Povidone	18300006	1
Caelo	Povidone	19127604	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Povidone	19175202	5
Caelo	Povidone	19175204	2
Caelo	Povidone	192500001	1
Caelo	Povidone	19500001	1
Caelo	Povidone	20000212001	10
Caelo	Povidone	20000212005	3
Caelo	Povidone	20001927003	1
Caelo	Povidone	20003415001	2
Caelo	Povidone	20003415004	1
Caelo	Povidone	20003415005	2
Caelo	Povidone	20003606003	1
Caelo	Povidone	21001192003	4
Caelo	Povidone	21001192005	1
Caelo	Povidone	21003749002	4
Caelo	Povidone	22001357001	4
Caesar & Loretz GmbH…	Povidone	20000212005	1
Caesar & Loretz GmbH…	Povidone	20003415005	1
Caesar & Loretz GmbH…	Povidone	20001927003	2
Caesar & Loretz GmbH…	Povidone	20003415001	1
Caesar & Loretz GmbH…	Povidone	20000212001	1
Caesar & Loretz GmbH…	Povidone	20003415001	4
Caesar & Loretz GmbH…	Povidone	20003415004	1
Caesar & Loretz GmbH…	Povidone	21001192003	1
Caesar & Loretz GmbH…	Povidone	21003749002	1
Caesar & Loretz GmbH/Sa	Povidone	20000212005	1
Caesar & Loretz GmbH	Povidone	18112201	1
Caesar & Loretz GmbH	Povidone	18238302	1
Caesar & Loretz GmbH	Povidone	18300002	2
Caesar & Loretz GmbH	Povidone	18300006	1
Caesar & Loretz GmbH	Povidone	19127604	1
Caesar & Loretz GmbH	Povidone	19175202	1
Caesar & Loretz GmbH	Povidone	20000212001	1
Caesar & Loretz GmbH	Povidone	20000212005	2
Caesar & Loretz GmbH	Povidone	20001927003	4
Caesar & Loretz GmbH	Povidone	20003415001	3
Caesar & Loretz GmbH	Povidone	20003415004	3
Caesar & Loretz GmbH	Povidone	20003415005	3
Caesar & Loretz GmbH	Povidone	20003606001	1
Caesar & Loretz GmbH	Povidone	21001192003	1
Caesar & Loretz GmbH	Povidone	21001192005	5
Caesar & Loretz GmbH	Povidone	21003749002	5
Caesar & Loretz GmbH	Povidone	22001357001	3
Caesar & Loretz Hild…	Povidone	18300002	1
Caesar / Ebert	Povidone	15383101	2
Cealo	Povidone	4369127	1
Fagron	Povidone	11276509T0	1
Fagron	Povidone	15C12-B02-327866	1
Fagron	Povidone	24701988Q0	1
GEHE	Povidone	18112201	1
Gehe	Povidone	18300002	1
Gehe	Povidone	22001357001	4
Phönix	Povidone	192500001	1
Sanacorp	Povidone	32470709T0	1

- 235 883 spectra from 1515 *Apo-Ident* customers from a total of 49 199 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Povidone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Povidone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	600	0	152 362
Type B	0	380	0	201 704
Type C	0	164	20	235 883

The substance/substance group *Povidone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.4211 %)
Type C	100.0000 % (> 99.9007 %)	89.1304 % (> 87.5000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20684	20684	0.00	30.73
20770	20770	0.00	52.35
21378	21378	0.00	29.27
22731	22731	0.00	89.50
23255	23255	0.00	31.30
23265	23265	0.00	72.30
24044	24044	0.00	35.81
24746	24746	0.00	114.25
24754	24754	0.00	140.77
25194	25194	0.00	144.21
25624	25624	0.00	83.54
26003	26003	0.00	81.64
26287	26831	17.97	51.11
26831	26831	0.00	53.74
27335	27335	0.00	94.94

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Povidone iodine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20472-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Povidone iodine; Povidonum iodinatum

Special notes

When selecting the *Povidone iodine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Povidone iodine	17	6	57

Second-stage model

For differentiation of the substance/substance group *Povidone iodine* the following second-stage model is used:

- Submodel 05

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Povidone iodine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Povidone	21.14	16.46
Fusidic acid	61.49	46.41
⋮	⋮	⋮
Progesterone	85.15	52.91
Spironolactone	>50	53.79
Testosterone propionate	>50	78.19
Ubidecarenone	>50	137.77

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Povidone iodine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Povidone iodine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Povidone iodine	13337205	21466	60	20131021
Caelo	Povidone iodine	15234101	23252	40	AR-17-FG-015433-02
Caelo	Povidone iodine	15234109	23256	40	20150717
Caelo	Povidone iodine	182385	24234	40	20180917*
Caelo	Povidone iodine	20003244	25659	40	20210106*
Caelo	Povidone iodine	22001868	26238	40	20220720*
Caelo	Povidone iodine	23000265	26725	40	20230331*
Euro OTC	Povidone iodine	1501029-01	21777	60	20150211
Euro OTC	Povidone iodine	1509009	21908	60	20150918*
Euro OTC	Povidone iodine	1606026-02	23906	40	20160708
Euro OTC	Povidone iodine	1805007	24118	40	20180525*
Euro OTC	Povidone iodine	1905008	24770	40	20190628*
Euro OTC	Povidone iodine	2001048	25122	40	20200320*
Euro OTC	Povidone iodine	2003030	25240	40	20200707*
Euro OTC	Povidone iodine	2009042	25433	40	20201022*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Povidone iodine	2206025	26225	40	20220721*
Euro OTC	Povidone iodine	2206025	26225SI	20	20220721*
Euro OTC	Povidone iodine	2305022	26750	40	20230705*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 760 spectra of 18 reference samples from the substance/substance group *Povidone iodine*. These samples are listed above in the *calibration samples* section. The reference samples come from 17 different batches.
- 152 202 spectra from a total of 2825 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 270 spectra of 8 reference samples from the substance/substance group *Povidone iodine*.
- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Povidone iodine	180763	24261	40
Caelo	Povidone iodine	192297	24879	40
Euro OTC	Povidone iodine	1606026	22675	40
Euro OTC	Povidone iodine	1704007	23435	40
Euro OTC	Povidone iodine	2202017	26044	40
Euro OTC	Povidone iodine	2406008	27295	40
Caelo	Povidone iodine	22001868	26238SI†	20
Euro OTC	Povidone iodine	2202017	26044SI	10

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 814 spectra from a total of 4038 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 199 spectra from 75 *Apo-Ident* customers from 63 batches from the substance/substance group *Povidone iodine*.
- Among them are spectra of independent samples from 57 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Povidone iodine	22001868001	2
	Povidone iodine	22001868004	2
	Povidone iodine	2206025	1
	Povidone iodine	2206025-01	2
apo-ident	Povidone iodine	1606026-02	1
Audor Pharma	Povidone iodine	2009042-01	1
BASF, Noweda	Povidone iodine	1110013-02	1
Basf/Sanacorp	Povidone iodine	180500701	1
Basf/Sanacorp	Povidone iodine	2009042-01	1
Caelo	Povidone iodine	1110013-02	1
Caelo	Povidone iodine	11168607	1
Caelo	Povidone iodine	11168612	1
Caelo	Povidone iodine	12072605	1
Caelo	Povidone iodine	12153106	2
Caelo	Povidone iodine	12153110	2
Caelo	Povidone iodine	12153116	2
Caelo	Povidone iodine	12153119	2
Caelo	Povidone iodine	1407032-01	1
Caelo	Povidone iodine	14195810	2
Caelo	Povidone iodine	1501029-01	3
Caelo	Povidone iodine	15121402	1
Caelo	Povidone iodine	15234101	1
Caelo	Povidone iodine	15234109	1
Caelo	Povidone iodine	15442405	1
Caelo	Povidone iodine	17028102	2
Caelo	Povidone iodine	18025301	1
Caelo	Povidone iodine	1805007-01	1
Caelo	Povidone iodine	18076308	1
Caelo	Povidone iodine	1905008-01	1
Caelo	Povidone iodine	19061302	1
Caelo	Povidone iodine	192297004	6
Caelo	Povidone iodine	20003244001	4
Caelo	Povidone iodine	20003244004	2
Caelo	Povidone iodine	21001575002	2
Caelo	Povidone iodine	21001575004	1
Caelo	Povidone iodine	22001868004	1
Caesar & Loretz GmbH...	Povidone iodine	19075002	1
Caesar & Loretz GmbH	Povidone iodine	18076308	1
Caesar & Loretz GmbH	Povidone iodine	19075003	1
Caesar & Loretz GmbH	Povidone iodine	192297002	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Povidone iodine	192297003	1
Caesar & Loretz GmbH	Povidone iodine	20003244001	4
Caesar & Loretz GmbH	Povidone iodine	20003244006	1
Caesar & Loretz GmbH	Povidone iodine	20004050001	1
Caesar & Loretz GmbH	Povidone iodine	2003244001	1
Caesar & Loretz GmbH	Povidone iodine	21001575002	1
EuRho/Noweda	Povidone iodine	1606026-02	5
EuRho/Noweda	Povidone iodine	2009042-02	1
EuRho	Povidone iodine	2003030-01	2
Euro OTC	Povidone iodine	110013-02	1
Euro OTC	Povidone iodine	111001302	1
Euro OTC	Povidone iodine	130901001	1
Euro OTC	Povidone iodine	1401029-01	1
Euro OTC	Povidone iodine	1407032-01	5
Euro OTC	Povidone iodine	1509009-01	2
Euro OTC	Povidone iodine	1509009-02	2
Euro OTC	Povidone iodine	1603023-01	2
Euro OTC	Povidone iodine	1606026	1
Euro OTC	Povidone iodine	1606026-02	12
Euro OTC	Povidone iodine	1704007-01	2
Euro OTC	Povidone iodine	1704007-02	2
Euro OTC	Povidone iodine	180500701	1
Euro OTC	Povidone iodine	1805007-01	7
Euro OTC	Povidone iodine	1805007-02	8
Euro OTC	Povidone iodine	1905008	1
Euro OTC	Povidone iodine	190500801	1
Euro OTC	Povidone iodine	1905008-01	26
Euro OTC	Povidone iodine	2001048-01	1
Euro OTC	Povidone iodine	2003030-01	10
Euro OTC	Povidone iodine	2009042-01	7
Euro OTC	Povidone iodine	2009042-02	5
Euro OTC	Povidone iodine	2202017-01	1
Euro OTC	Povidone iodine	2206025-01	1
Euro OTC	Povidone iodine	8051808	1
Euro OTC	Povidone iodine	G4208BPZ0	2
Euro/ Jenne	Povidone iodine	1606026-02	4
Euroo/Phoenix	Povidone iodine	G3115BPZ0	1
Fagron	Povidone iodine	1110013-02	1
Noweda	Povidone iodine	G0354BPZ0	1
ph euro	Povidone iodine	19050080-01	1
Phoenix	Povidone iodine	2003030-01	1
Phönix	Povidone iodine	1110013-02	1
Sanacorp	Povidone iodine	1110013-02	4
Sanacorp	Povidone iodine	2202017-01	1
Sanacorp	Povidone iodine	2406008-01	1
Stumpf	Povidone iodine	11168612	1

- 235 868 spectra from 1515 *Apo-Ident* customers from a total of 49 196 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Povidone iodine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Povidone iodine* and it was evaluated

how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	760	0	152 202
Type B	0	265	5	201 814
Type C	0	188	11	235 868

The substance/substance group *Povidone iodine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.2105 %)
Type B	100.0000 % (> 99.9912 %)	98.1481 % (> 97.0370 %)
Type C	100.0000 % (> 99.9007 %)	94.4724 % (> 92.9648 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21466	21908	7.66	49.97
21777	21908	6.48	52.17
21908	21908	0.00	59.71
23252	23252	0.00	56.99
23256	23252	15.08	53.49
23906	21908	11.67	47.15
24118	24118	0.00	159.21
24234	24234	0.00	50.05
24770	24770	0.00	52.72
25122	25122	0.00	47.04
25240	25240	0.00	49.49
25433	25433	0.00	49.62
25659	25659	0.00	48.24
26225	26225	0.00	55.76
26238	26238	0.00	151.69
26725	26725	0.00	135.50
26750	26750	0.00	26.56

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Prasterone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20703-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Prasterone; Prasteronum

Special notes

When selecting the *Prasterone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Prasterone	21	18	125

Second-stage model

For differentiation of the substance/substance group *Prasterone* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Prasterone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Estradiol valerate	86.83	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Prasterone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Prasterone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Prasterone	APZDHA16003-M	23931	40	1805404
Audor Pharma	Prasterone	APZDHAC17003MD	24412	40	20180119
Audor Pharma	Prasterone	APZDHAC18004D	24430	40	1906523
Euro OTC	Prasterone	1102036-01	20703	40	1404310
Euro OTC	Prasterone	1506011	21824	60	20150629*
Euro OTC	Prasterone	1602018	22506	30	20160301*
Euro OTC	Prasterone	1704012	23389	40	20170529*
Euro OTC	Prasterone	1707014	23695	40	20170829*
Euro OTC	Prasterone	1710035	23868	40	20171212*
Euro OTC	Prasterone	1712014	23893	40	20180115*
Euro OTC	Prasterone	1809009	24323	40	20181010*
Euro OTC	Prasterone	1907045	24853	40	20190905*
Euro OTC	Prasterone	1809009	24966	40	20191111*
Euro OTC	Prasterone	1910025	24967	40	20191111*
Euro OTC	Prasterone	2001038	25091	40	20200302*
Euro OTC	Prasterone	2102004	25537	40	20210224*
Euro OTC	Prasterone	2101011	25568	40	20210224*
Euro OTC	Prasterone	2301032	26513	39	20230202*
Fagron	Prasterone	13J10-B02-287175	20960	40	1404309
Fagron	Prasterone	15G14-B07-310827	21917	60	20150814
Fagron	Prasterone	16L13-B01-330724	23865	40	20161228
Fagron	Prasterone	22E25-F01-382686	26408	40	20220720

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 909 spectra of 22 reference samples from the substance/substance group *Prasterone*. These samples are listed above in the *calibration samples* section. The reference samples come from 21 different batches.
- 152 053 spectra from a total of 2821 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 800 spectra of 23 reference samples from the substance/substance group *Prasterone*.
- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Audor Pharma	Prasterone	APZDHA16003-1MD	23932	40
Euro OTC	Prasterone	1702025	23147	40
Euro OTC	Prasterone	1805018	24137	40
Euro OTC	Prasterone	1809010	24318	40
Euro OTC	Prasterone	1901030	24453	40
Euro OTC	Prasterone	1901031	24454	40
Euro OTC	Prasterone	2005008	25152	40
Euro OTC	Prasterone	2005007	25153	40
Euro OTC	Prasterone	2201038	25955	40
Euro OTC	Prasterone	2203004	26100	30
Euro OTC	Prasterone	2206014	26216	40
Euro OTC	Prasterone	2209007	26344	40
Euro OTC	Prasterone	2301031	26594	40
Euro OTC	Prasterone	2311028	27003	40
Euro OTC	Prasterone	2408001	27393	40
Euro OTC	Prasterone	2408002	27394	40
Fagron	Prasterone	18C12-B01-347633	23990	40
Fagron	Prasterone	23K03-B04-231722	27033	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Prasterone	2201038	25955SI	10
Euro OTC	Prasterone	2203004	26100SI	20
Euro OTC	Prasterone	2206014	26216SI	20
Euro OTC	Prasterone	2209007	26344SI	20
Fagron	Prasterone	22E25-F01-382686	26408SI[†]	20

- 201 284 spectra from a total of 4026 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 264 spectra from 67 *Apo-Ident* customers from 128 batches from the substance/substance group *Prasterone*.
- Among them are spectra of independent samples from 125 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Prasterone	2206014-01	1
	Prasterone	22A17-F01-381261	1
	Prasterone	22E25-F01-382686	1
	Prasterone	2301031	1
	Prasterone	2301031-01	1
	Prasterone	2301032-01	2
	Prasterone	2301032-02	5
	Prasterone	2311028-01	1
	Prasterone	23K03-B04-231723	1
	Prasterone	23L01-B05-231787	1
	Prasterone	23L01-B05-238894	1
Audor Pharma	Prasterone	10050051/1P	1
Audor Pharma	Prasterone	AP11040002P	2
Audor Pharma	Prasterone	AP5103540P	1
Audor Pharma	Prasterone	APTDHAC17003-MD	3
Audor Pharma	Prasterone	APZDHA16003-M	1
Audor Pharma	Prasterone	APZDHAC17003-MD	3
Caelo	Prasterone	1412028-01	1
Caelo	Prasterone	15A15-B40-307323	1
Caelo	Prasterone	16B19-B04-318665	1
Caelo	Prasterone	16I02-B02-326485	1
Caelo	Prasterone	16l02-B02-326485	2
EuRho/Gehe	Prasterone	2005007-01	1
EuRho/Noweda	Prasterone	2101011-02	1
EuRho	Prasterone	1311002-01	1
Euro OTC	Prasterone	1306021-01	3
Euro OTC	Prasterone	1311002-01	2
Euro OTC	Prasterone	1401040-01	1
Euro OTC	Prasterone	1409004-01	4
Euro OTC	Prasterone	1412028	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Prasterone	1412028-01	4
Euro OTC	Prasterone	1506011-01	4
Euro OTC	Prasterone	1602018-01	5
Euro OTC	Prasterone	1602018-02	2
Euro OTC	Prasterone	1702025	3
Euro OTC	Prasterone	170202501	1
Euro OTC	Prasterone	1702025-01	7
Euro OTC	Prasterone	1704012-01	1
Euro OTC	Prasterone	18050118-01	1
Euro OTC	Prasterone	1805018-01	4
Euro OTC	Prasterone	1809009-01	1
Euro OTC	Prasterone	1809009-03	6
Euro OTC	Prasterone	180901001	1
Euro OTC	Prasterone	1809010-01	4
Euro OTC	Prasterone	1901030-01	1
Euro OTC	Prasterone	1901030-02	1
Euro OTC	Prasterone	190103101	1
Euro OTC	Prasterone	1901031-01	3
Euro OTC	Prasterone	1901031-02	1
Euro OTC	Prasterone	1910025-01	3
Euro OTC	Prasterone	2001038-01	6
Euro OTC	Prasterone	200500701	1
Euro OTC	Prasterone	2005007-01	4
Euro OTC	Prasterone	2005008-01	11
Euro OTC	Prasterone	201101	2
Euro OTC	Prasterone	2081302	1
Euro OTC	Prasterone	2101011-02	7
Euro OTC	Prasterone	2101011-03	6
Euro OTC	Prasterone	2102004-02	2
Euro OTC	Prasterone	2102004-03	4
Euro OTC	Prasterone	2102004-04	1
Euro OTC	Prasterone	220103801	1
Euro OTC	Prasterone	2201038-01	7
Euro OTC	Prasterone	22021306	1
Euro OTC	Prasterone	2203004-01	1
Euro OTC	Prasterone	2206014-01	1
Euro OTC	Prasterone	220900701	1
Euro OTC	Prasterone	2209007-01	1
Euro OTC	Prasterone	23021711	1
Euro OTC	Prasterone	26031506	1
Euro OTC	Prasterone	30041509	1
Euro OTC	Prasterone	4091511	1
Euro OTC	Prasterone	5101849	1
Euro OTC	Prasterone	9215-4/09	1
Euro OTC	Prasterone	DHEA150801-1	1
Euro OTC	Prasterone	T03-04/1412028-01	1
Euro OTC	Prasterone	XPC0263	1
Euro OTC	Prasterone	ZDHAC18002	1
Euro/AHD	Prasterone	2005007-01	3
Euro/AHD	Prasterone	2102004-04	1
Fagron	Prasterone	12C26-N09	1
Fagron	Prasterone	12G04-N19	2
Fagron	Prasterone	12K30-N06	3
Fagron	Prasterone	13J10-B02	1
Fagron	Prasterone	13J10-B02-287177	1
Fagron	Prasterone	1421-B03-300211	1
Fagron	Prasterone	14C18-B02	1
Fagron	Prasterone	14c18b02293602	1
Fagron	Prasterone	14C18-B02-293602	1
Fagron	Prasterone	14C18-B02-293606	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prasterone	14C18-Bo2-293603	1
Fagron	Prasterone	14h12b05-297723	1
Fagron	Prasterone	14H12-B05-297727	2
Fagron	Prasterone	15A15-B40-307323	1
Fagron	Prasterone	15G14-B07-310827	1
Fagron	Prasterone	15I18-B09-316798	1
Fagron	Prasterone	16B19-B04-318665	2
Fagron	Prasterone	16B19-B04-322246	2
Fagron	Prasterone	16IO2-B02-326485	2
Fagron	Prasterone	16J26-B03-327602	1
Fagron	Prasterone	16L13-B01-332104	1
Fagron	Prasterone	17D11-B10-336395	1
Fagron	Prasterone	18B02-B02-345147	1
Fagron	Prasterone	18B13-B09_346424	1
Fagron	Prasterone	18C12	1
Fagron	Prasterone	18E15-B03-350802	2
Fagron	Prasterone	19061304	1
Fagron	Prasterone	19G10-B02-365017	2
Fagron	Prasterone	19G10-B02-365018	1
Fagron	Prasterone	19G10-B02-365154	2
Fagron	Prasterone	19G10-B02-365155	1
Fagron	Prasterone	20123-F03-374815	2
Fagron	Prasterone	20C25-U03-005782	1
Fagron	Prasterone	20I23-F03-374815	1
Fagron	Prasterone	20l23-F03-374815	1
Fagron	Prasterone	21G13-F03-380169	6
Fagron	Prasterone	21G13-F03-380169	1
Fagron	Prasterone	22A17-F01-381262	1
Fagron	Prasterone	22H22-B04-223769	1
Fagron	Prasterone	22K21-B05-225380	1
Fagron	Prasterone	27071705	1
Fagron	Prasterone	7013260004	1
Fagron	Prasterone	701326-0005	1
Fagron	Prasterone	C04-140804(M)	1
Fagron	Prasterone	DHEA160802	1
Fagron	Prasterone	DHEA190504	2
Fagron	Prasterone	DHEAA150401-1	1
Fagron	Prasterone	DHEAH200604W	2
Fagron	Prasterone	F02-3779709	1
Fargon	Prasterone	16B19-B04-318665	1
Fragon	Prasterone	12G04-N19	1
Gall Pharma	Prasterone	16/02-B02	1
Gehe	Prasterone	2005007-01	2
Gehe	Prasterone	2102004-02	2
Haihang Industry	Prasterone	20130816	4
Haihang	Prasterone	20130507	1
Jacoby Gatt-Koller	Prasterone	20J02359	1
Kögl	Prasterone	1803108	1
Nachprüfung	Prasterone	120022	1
NWM Shandong Northwe…	Prasterone	PST151207	1
Ph.Eur/AHD	Prasterone	1809009-03	1
Phönix	Prasterone	2102004-04	4
PROQUINA	Prasterone	1602018_02	1
Sanacorp	Prasterone	1805018-01	1
Sanacorp	Prasterone	2203004-01	1

- 235 803 spectra from 1515 *Apo-Ident* customers from a total of 49 131 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Prasterone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prasterone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	909	0	152 053
Type B	0	800	0	201 284
Type C	0	264	0	235 803

The substance/substance group *Prasterone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.3399 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2500 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 97.7273 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20703	20703	0.00	149.79
20960	20960	0.00	149.04
21824	21824	0.00	143.19
21917	25091	26.60	143.38
22506	22506	0.00	152.62
23389	23389	0.00	108.92
23695	23695	0.00	122.12
23865	23695	43.72	137.04
23868	23868	0.00	111.98
23893	23893	0.00	134.02
23931	23931	0.00	138.91
24323	24323	0.00	138.36
24412	23893	6.84	133.77

continued on the next page

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24430	24430	0.00	116.37
24853	24853	0.00	140.32
24966	24966	0.00	148.99
24967	24967	0.00	147.68
25091	25091	0.00	146.98
25537	25537	0.00	149.88
25568	25568	0.00	148.40
26408	25091	15.42	150.52
26513	26513	0.00	145.96

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Praziquantel**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	24840-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Praziquantel; Praziquantelum

Special notes

When selecting the *Praziquantel* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Praziquantel	3	1	0

Second-stage model

For differentiation of the substance/substance group *Praziquantel* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Praziquantel* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ofloxacin	82.57	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Praziquantel* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Praziquantel*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Praziquantel	2205031	26185	40	20220620*
Euro OTC	Praziquantel	2205031	26185SI	20	20220620*
Euro OTC	Praziquantel	2401015	27159	30	20240227*
Euro OTC	Praziquantel	2402035	27162	40	20240313*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 130 spectra of 4 reference samples from the substance/substance group *Praziquantel*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 832 spectra from a total of 2839 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 3 reference samples from the substance/substance group *Praziquantel*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Praziquantel	1908004	24840	40
Euro OTC	Praziquantel	2401015	27159SI†	20
Euro OTC	Praziquantel	2402035	27162SI†	20

- 202 004 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Praziquantel*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Validation results

The validation runs checked whether the substance/substance group *Praziquantel* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Praziquantel* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	130	0	152 832
Type B	0	80	0	202 004
Type C	0	0	0	236 067

The substance/substance group *Praziquantel* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.3846 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26185	26185	0.00	104.62
27159	27159	0.00	104.31
27162	27162	0.00	102.70

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Prednicarbate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20196-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Prednicarbate; Prednicarbatum

Special notes

When selecting the *Prednicarbate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Prednicarbate	13	18	494

Second-stage model

For differentiation of the substance/substance group *Prednicarbate* the following second-stage model is used:

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Prednicarbate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prednisolon dihydrogen phosphate di…	48.83	–
Ciclosporin	111.03	–
⋮	⋮	⋮
Oxybutynin hydrochloride	>50	63.41
Levocarnitine	>50	146.11
Capsaicin	>50	149.61
Sodium citrate	>50	160.35
Cyproterone acetate	>50	191.37
Tetracaine	>50	217.19
Norethisterone acetate	>50	224.58
Amitriptyline hydrochloride	>50	328.16
Quinine hydrochloride dihydrate	>50	411.25
Heparin sodium	>50	428.04
Alfatradiol	>50	529.52
Pyridoxal-5-phosphate	>50	584.42
Valine	>50	610.65
Methoxsalen	>50	627.94
Ciprofloxacin hydrochloride	>50	635.05
Sucrose	>50	1932.95
Amifampridine	>50	2013.98
Triclosan	>50	2054.82

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Prednicarbate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Prednicarbate*:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Prednicarbate	13119402	20832	60	1501576
Caelo	Prednicarbate	13119402	20833	60	20130517
Caelo	Prednicarbate	13119402	20833SI	30	20130517
Caelo	Prednicarbate	13372404	21368	50	AR-15-FG-007941-02
Caelo	Prednicarbate	13372404	21369	49	20131119
Caelo	Prednicarbate	13372404	21369SI	33	20131119
Euro OTC	Prednicarbate	1302033-02	21610	60	1509286
Euro OTC	Prednicarbate	1507011	21858	60	20150730*
Euro OTC	Prednicarbate	1601058	22366	45	20160223*
Euro OTC	Prednicarbate	1601058	22366SI	31	20160223*
Euro OTC	Prednicarbate	2001031	25119	40	20200331*
Euro OTC	Prednicarbate	2009018	25401	40	20200930*
Euro OTC	Prednicarbate	2103017	25609	40	20210408*
Euro OTC	Prednicarbate	2103017	25609SI	38	20210408*
Euro OTC	Prednicarbate	2204014	26084	40	20220511*
Euro OTC	Prednicarbate	2405019	27277	40	20240704*
Euro OTC	Prednicarbate	2405019	27277SI	30	20240704*
Fagron	Prednicarbate	12D27-N04	20700	40	20120509
Fagron	Prednicarbate	12D27-N04	20700SI	48	20120509
Fagron	Prednicarbate	14A27-B02-291256	21572	60	AR-16-FG-011442-01
Fagron	Prednicarbate	22F03-B02-223103	26393	40	20220930
Fagron	Prednicarbate	22F03-B02-223103	26393SI	30	20220930

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 964 spectra of 22 reference samples from the substance/substance group *Prednicarbate*. These samples are listed above in the *calibration samples* section. The reference samples come from 13 different batches.
- 151 998 spectra from a total of 2829 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1297 spectra of 41 reference samples from the substance/substance group *Prednicarbate*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Prednicarbate	160874	22447	60
Caelo	Prednicarbate	170138	23040	40
Caelo	Prednicarbate	173156	23845	40
Caelo	Prednicarbate	172204	23848	40
Caelo	Prednicarbate	21001161001	25928	40
Caelo	Prednicarbate	22000755	26130	40
Caelo	Prednicarbate	23001025	26847	40
Caelo	Prednicarbate	23001026	26848	40
Euro OTC	Prednicarbate	1605001	22558	30
Euro OTC	Prednicarbate	1607012	22703	40
Euro OTC	Prednicarbate	1609022	22860	40
Euro OTC	Prednicarbate	1707022	23540	40
Euro OTC	Prednicarbate	1801013	23887	40
Euro OTC	Prednicarbate	1805005	24134	40
Euro OTC	Prednicarbate	1809015	24320	40
Euro OTC	Prednicarbate	1903023	24633	40
Euro OTC	Prednicarbate	2304020	26922	40
Euro OTC	Prednicarbate	2411003	27458	30
Caelo	Prednicarbate	160874	22447SI	30
Caelo	Prednicarbate	170138	23040SI	20
Caelo	Prednicarbate	173156	23845SI	20
Caelo	Prednicarbate	172204	23848SI	20
Caelo	Prednicarbate	21001161001	25928SI	36
Caelo	Prednicarbate	22000755	26130SI	30
Caelo	Prednicarbate	23001025	26847SI	30
Caelo	Prednicarbate	23001026	26848SI	30
Euro OTC	Prednicarbate	1507011	21858SI†	15
Euro OTC	Prednicarbate	1605001	22558SI	25
Euro OTC	Prednicarbate	1607012	22703SI	28
Euro OTC	Prednicarbate	1609022	22860SI	27
Euro OTC	Prednicarbate	1707022	23540SI	19
Euro OTC	Prednicarbate	1801013	23887SI	20
Euro OTC	Prednicarbate	1805005	24134SI	20
Euro OTC	Prednicarbate	1809015	24320SI	20
Euro OTC	Prednicarbate	1903023	24633SI	32
Euro OTC	Prednicarbate	2001031	25119SI†	27
Euro OTC	Prednicarbate	2009018	25401SI†	25
Euro OTC	Prednicarbate	2204014	26084SI†	10
Euro OTC	Prednicarbate	2304020	26922SI	37
Euro OTC	Prednicarbate	2411003	27458SI	20
Fagron	Prednicarbate	14A27-B02-291256	21572SI†	36

- 200 787 spectra from a total of 4022 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

provided by the customer regarding manufacturer and batch number.

- 3979 spectra from 1071 *Apo-Ident* customers from 515 batches from the substance/substance group *Prednicarbate*.
- Among them are spectra of independent samples from 492 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Prednicarbate	2001031-01	1
	Prednicarbate	21000991002	1
	Prednicarbate	21001161004	1
	Prednicarbate	21001161006	1
	Prednicarbate	21001161011	1
	Prednicarbate	2103017-01	3
	Prednicarbate	21F07-B17-216553	1
	Prednicarbate	22000755001	6
	Prednicarbate	22000755002	2
	Prednicarbate	22000755003	1
	Prednicarbate	22000755005	3
	Prednicarbate	22000755007	5
	Prednicarbate	22000755008	5
	Prednicarbate	22000755009	13
	Prednicarbate	22000755010	6
	Prednicarbate	2200755002	2
	Prednicarbate	220401401	2
	Prednicarbate	2204014-01	13
	Prednicarbate	2204014-02	1
	Prednicarbate	22F03-B02_223103	1
	Prednicarbate	22F03-B02-218938	1
	Prednicarbate	22F03-B02-223102	5
	Prednicarbate	22F03-B02-223103	2
	Prednicarbate	22F03-B02-223104	1
	Prednicarbate	22F03-B02-2277918	1
	Prednicarbate	22F03-B02-227918	4
	Prednicarbate	22F03-B02-227919	2
	Prednicarbate	22F03-B02-232393	2
	Prednicarbate	23001025003	3
	Prednicarbate	23001026001	26
	Prednicarbate	23001026002	23
	Prednicarbate	23001026003	3
	Prednicarbate	23003318001	1
	Prednicarbate	2304020_01	1
	Prednicarbate	2304020-01	15
	Prednicarbate	2304040-01	1
	Prednicarbate	23H24-B06-232394	2
	Prednicarbate	B06-2323904	1
19Caesar & Loretz GmbH	Prednicarbate	22000755001	1
AEP	Prednicarbate	19E14-B01-191430	3
AEP	Prednicarbate	21000991003	1
AEP	Prednicarbate	22000755003	1
AHC	Prednicarbate	20000609004	1
AHC	Prednicarbate	20000609009	1
AHC	Prednicarbate	20003660005	2
AHC	Prednicarbate	2009018-01	1
AHD	Prednicarbate	17220408	1
AHD	Prednicarbate	1801013-01	1
AHD	Prednicarbate	1809015-01	1
AHD	Prednicarbate	21001161001	1
AHD	Prednicarbate	21001161006	1
AHD	Prednicarbate	21K24-B03-213699	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
AHD	Prednicarbate	2204014-01	1
AHD	Prednicarbate	23001026001	1
AHD	Prednicarbate	23001026003	1
AHD	Prednicarbate	23003318001	1
AHD	Prednicarbate	2304020-01	1
AHL	Prednicarbate	16087408	2
Alliance Healthcare	Prednicarbate	21001161010	1
Alliance Healthcare	Prednicarbate	22000755002	1
Alliance Healthcare	Prednicarbate	22000755003	1
Alliance Healthcare	Prednicarbate	2204014-01	1
Alliance	Prednicarbate	22000755002	1
Alliance	Prednicarbate	22000755010	1
Anzag	Prednicarbate	17220408	1
Apo-ident/Phoenix	Prednicarbate	1903023-01	1
apo-ident	Prednicarbate	1607012-01	1
apomix	Prednicarbate	13372410	2
apomix	Prednicarbate	1609022-01	2
Bombastus	Prednicarbate	15446306	1
Bombastus	Prednicarbate	17220408	1
Bombastus	Prednicarbate	17315605	1
Caelo	Prednicarbate		3
Caelo	Prednicarbate	118194105	1
Caelo	Prednicarbate	11L23-N07	2
Caelo	Prednicarbate	12(20000609009)	1
Caelo	Prednicarbate	121223613	1
Caelo	Prednicarbate	12123610	1
Caelo	Prednicarbate	1213608	1
Caelo	Prednicarbate	1220218/17220407	1
Caelo	Prednicarbate	12383301	1
Caelo	Prednicarbate	12383309	1
Caelo	Prednicarbate	13(20003660005)	1
Caelo	Prednicarbate	13/23-N04	1
Caelo	Prednicarbate	13119401	1
Caelo	Prednicarbate	13119402	2
Caelo	Prednicarbate	13224401	5
Caelo	Prednicarbate	13224406	2
Caelo	Prednicarbate	13372403	11
Caelo	Prednicarbate	13372408	1
Caelo	Prednicarbate	13372410	6
Caelo	Prednicarbate	13372411	1
Caelo	Prednicarbate	13372419	6
Caelo	Prednicarbate	14(20003660008)	1
Caelo	Prednicarbate	14A27-B02-295796	1
Caelo	Prednicarbate	14A27-B02-295797	1
Caelo	Prednicarbate	14J16-B06	3
Caelo	Prednicarbate	15(21000991002)	1
Caelo	Prednicarbate	1507011-01	1
Caelo	Prednicarbate	1517E-03595	1
Caelo	Prednicarbate	15181403	13
Caelo	Prednicarbate	15181404	3
Caelo	Prednicarbate	15181408	1
Caelo	Prednicarbate	15181409	4
Caelo	Prednicarbate	15181411	2
Caelo	Prednicarbate	15446301	22
Caelo	Prednicarbate	15446302	13
Caelo	Prednicarbate	15446303	3
Caelo	Prednicarbate	1544630306	1
Caelo	Prednicarbate	15446304	1
Caelo	Prednicarbate	15446305	6
Caelo	Prednicarbate	15446306	13

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednicarbate	15D15-B03	1
Caelo	Prednicarbate	15D15-B03-308161	1
Caelo	Prednicarbate	15D15-B03-310847	2
Caelo	Prednicarbate	15G10-B02-314082	3
Caelo	Prednicarbate	15J22-B04-318528	1
Caelo	Prednicarbate	15J22-B-321005	1
Caelo	Prednicarbate	1601058-01	1
Caelo	Prednicarbate	160500	1
Caelo	Prednicarbate	1605001	1
Caelo	Prednicarbate	160701201	1
Caelo	Prednicarbate	1607012-01	2
Caelo	Prednicarbate	1608710	1
Caelo	Prednicarbate	16087401	13
Caelo	Prednicarbate	16087408	20
Caelo	Prednicarbate	16087410	22
Caelo	Prednicarbate	16087411	3
Caelo	Prednicarbate	16087412	6
Caelo	Prednicarbate	1609022-01	3
Caelo	Prednicarbate	168087410	1
Caelo	Prednicarbate	16987410	1
Caelo	Prednicarbate	16A18-B01-322732	1
Caelo	Prednicarbate	16A18-B01-322733	2
Caelo	Prednicarbate	16E12-B01	1
Caelo	Prednicarbate	16E12-B01-325758	1
Caelo	Prednicarbate	16J27-B01	1
Caelo	Prednicarbate	16J27-B01-330976	3
Caelo	Prednicarbate	16J27-B01-330977	1
Caelo	Prednicarbate	16J27-B01-332958	1
Caelo	Prednicarbate	17013804	14
Caelo	Prednicarbate	17013805	11
Caelo	Prednicarbate	17014001	3
Caelo	Prednicarbate	17014003	28
Caelo	Prednicarbate	17014005	20
Caelo	Prednicarbate	17014006	2
Caelo	Prednicarbate	1704003	1
Caelo	Prednicarbate	1704005	1
Caelo	Prednicarbate	1707022-01	3
Caelo	Prednicarbate	17220401	6
Caelo	Prednicarbate	17220406	4
Caelo	Prednicarbate	17220407	46
Caelo	Prednicarbate	1722040716J27-B01-33	1
Caelo	Prednicarbate	172204075515	1
Caelo	Prednicarbate	17220408	48
Caelo	Prednicarbate	17220410	2
Caelo	Prednicarbate	1722401	1
Caelo	Prednicarbate	173156	1
Caelo	Prednicarbate	17315603	7
Caelo	Prednicarbate	17315604	38
Caelo	Prednicarbate	17315605	28
Caelo	Prednicarbate	17315606	1
Caelo	Prednicarbate	17315607	2
Caelo	Prednicarbate	17315609	46
Caelo	Prednicarbate	17315611	3
Caelo	Prednicarbate	177220407	1
Caelo	Prednicarbate	17C27-B01-339079	1
Caelo	Prednicarbate	17J04-B05-343934	1
Caelo	Prednicarbate	17j04B05346113	1
Caelo	Prednicarbate	17J04-B05-346113	1
Caelo	Prednicarbate	180101301	1
Caelo	Prednicarbate	1801013-01	6

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednicarbate	1805005-01	1
Caelo	Prednicarbate	1814112	1
Caelo	Prednicarbate	1819104	1
Caelo	Prednicarbate	18194101	1
Caelo	Prednicarbate	18194103	12
Caelo	Prednicarbate	18194104	61
Caelo	Prednicarbate	18194105	80
Caelo	Prednicarbate	18194112	9
Caelo	Prednicarbate	18194115	48
Caelo	Prednicarbate	18194116	5
Caelo	Prednicarbate	18194117	21
Caelo	Prednicarbate	18194194	1
Caelo	Prednicarbate	18197115	1
Caelo	Prednicarbate	18294103	1
Caelo	Prednicarbate	18B27-B01-350264	2
Caelo	Prednicarbate	18E14-B03-352560	2
Caelo	Prednicarbate	18E14-B03-355726	1
Caelo	Prednicarbate	18E14-B03-355727	1
Caelo	Prednicarbate	19051601	57
Caelo	Prednicarbate	19051602	47
Caelo	Prednicarbate	1905-1602	1
Caelo	Prednicarbate	19051603	1
Caelo	Prednicarbate	19051604	9
Caelo	Prednicarbate	191122608	1
Caelo	Prednicarbate	19122602	18
Caelo	Prednicarbate	19122604	53
Caelo	Prednicarbate	19122608	53
Caelo	Prednicarbate	1922604	2
Caelo	Prednicarbate	1922608	1
Caelo	Prednicarbate	19G09-B01-194722	2
Caelo	Prednicarbate	2(18194104)	1
Caelo	Prednicarbate	200000609004	2
Caelo	Prednicarbate	20000360007	1
Caelo	Prednicarbate	200003660006	2
Caelo	Prednicarbate	200003660007	3
Caelo	Prednicarbate	20000609001	14
Caelo	Prednicarbate	20000609003	1
Caelo	Prednicarbate	20000609004	57
Caelo	Prednicarbate	20000609006	12
Caelo	Prednicarbate	20000609008	1
Caelo	Prednicarbate	20000609009	37
Caelo	Prednicarbate	2000060904	1
Caelo	Prednicarbate	20000609606	1
Caelo	Prednicarbate	2000360009	1
Caelo	Prednicarbate	20003660002	1
Caelo	Prednicarbate	20003660004	10
Caelo	Prednicarbate	20003660005	12
Caelo	Prednicarbate	20003660006	22
Caelo	Prednicarbate	20003660007	30
Caelo	Prednicarbate	200036600078	1
Caelo	Prednicarbate	20003660008	34
Caelo	Prednicarbate	20003660008mul	1
Caelo	Prednicarbate	20003660009	31
Caelo	Prednicarbate	2000366005	1
Caelo	Prednicarbate	2000366006	1
Caelo	Prednicarbate	2000366007	3
Caelo	Prednicarbate	2000366008	3
Caelo	Prednicarbate	2000366009	1
Caelo	Prednicarbate	200036660008	1
Caelo	Prednicarbate	20006069006	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednicarbate	2000609004	1
Caelo	Prednicarbate	2001031-01	5
Caelo	Prednicarbate	2003660007	1
Caelo	Prednicarbate	2003660008	2
Caelo	Prednicarbate	2003666009	1
Caelo	Prednicarbate	2009018-01	5
Caelo	Prednicarbate	2009018-02	1
Caelo	Prednicarbate	201372	1
Caelo	Prednicarbate	2018821009912	1
Caelo	Prednicarbate	20A21-B12	1
Caelo	Prednicarbate	2100091003	2
Caelo	Prednicarbate	21000991001	2
Caelo	Prednicarbate	21000991002	45
Caelo	Prednicarbate	21000991003	34
Caelo	Prednicarbate	21000991004	2
Caelo	Prednicarbate	21000991005	8
Caelo	Prednicarbate	2100116007	2
Caelo	Prednicarbate	21001161001	48
Caelo	Prednicarbate	21001161003	2
Caelo	Prednicarbate	21001161004	3
Caelo	Prednicarbate	21001161006	31
Caelo	Prednicarbate	21001161007	28
Caelo	Prednicarbate	21001161008	4
Caelo	Prednicarbate	21001161010	17
Caelo	Prednicarbate	21001161011	20
Caelo	Prednicarbate	21001161013	5
Caelo	Prednicarbate	2100161001	3
Caelo	Prednicarbate	2100161006	1
Caelo	Prednicarbate	2100161007	4
Caelo	Prednicarbate	2100991003	3
Caelo	Prednicarbate	2101161011	1
Caelo	Prednicarbate	2103017-01	2
Caelo	Prednicarbate	210906(21000991002)	1
Caelo	Prednicarbate	211001161011	1
Caelo	Prednicarbate	211007	1
Caelo	Prednicarbate	21990000022000	1
Caelo	Prednicarbate	21F07-817-216553	1
Caelo	Prednicarbate	21F07-B17-216554	1
Caelo	Prednicarbate	22000755001	13
Caelo	Prednicarbate	22000755002	10
Caelo	Prednicarbate	22000755003	15
Caelo	Prednicarbate	22000755005	3
Caelo	Prednicarbate	22000755006	2
Caelo	Prednicarbate	22000755007	9
Caelo	Prednicarbate	22000755009	1
Caelo	Prednicarbate	2200075509	2
Caelo	Prednicarbate	220075507	1
Caelo	Prednicarbate	22007553003	1
Caelo	Prednicarbate	220516(21001161010)	1
Caelo	Prednicarbate	23001026001	4
Caelo	Prednicarbate	23051819	1
Caelo	Prednicarbate	23082013A	1
Caelo	Prednicarbate	2748	1
Caelo	Prednicarbate	2790	1
Caelo	Prednicarbate	2x21001161001	1
Caelo	Prednicarbate	3(19051602)	1
Caelo	Prednicarbate	3267	1
Caelo	Prednicarbate	3272	1
Caelo	Prednicarbate	3302	1
Caelo	Prednicarbate	3438	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednicarbate	6090092	1
Caelo	Prednicarbate	718A-03595	1
Caelo	Prednicarbate	9764897	1
Caelo	Prednicarbate	C0333/1111070	2
Caelo	Prednicarbate	PNC101/0720	1
Caeol/Noweda	Prednicarbate	16A18-B01-322732	1
Caeol/Noweda	Prednicarbate	17315609	1
Caeol/Phornix	Prednicarbate	17315604	1
Caersar & Loretz	Prednicarbate	21000991002	1
Caesar & Lorenz GmbH	Prednicarbate	19051601	1
Caesar & Lorenz GmbH	Prednicarbate	19051602	1
Caesar & Loretz GmbH...	Prednicarbate	19051601	1
Caesar & Loretz GmbH...	Prednicarbate	21001161004	1
Caesar & Loretz GmbH...	Prednicarbate	21001161007	3
Caesar & Loretz GmbH...	Prednicarbate	18194112	1
Caesar & Loretz GmbH...	Prednicarbate	21000991002	1
Caesar & Loretz GmbH...	Prednicarbate	20003660009	1
Caesar & Loretz GmbH...	Prednicarbate	20000609009	1
Caesar & Loretz GmbH/ AHD	Prednicarbate	22000755003	1
Caesar & Loretz GmbH...	Prednicarbate	20000609004	1
Caesar & Loretz GmbH...	Prednicarbate	21001161007	1
Caesar & Loretz GmbH...	Prednicarbate	21001161010	1
Caesar & Loretz GmbH...	Prednicarbate	21001161011	1
Caesar & Loretz GmbH/AHD	Prednicarbate	20000609004	1
Caesar & Loretz GmbH/AHD	Prednicarbate	21001161010	1
Caesar & Loretz GmbH/E	Prednicarbate	21000991003	1
Caesar & Loretz GmbH...	Prednicarbate	1203584	1
Caesar & Loretz GmbH...	Prednicarbate	19122608	1
Caesar & Loretz GmbH...	Prednicarbate	21001161007	1
Caesar & Loretz GmbH...	Prednicarbate	B12-1975501	1
Caesar & Loretz GmbH/G	Prednicarbate	20003660009	1
Caesar & Loretz GmbH/G	Prednicarbate	21001161006	1
Caesar & Loretz GmbH/Gehe	Prednicarbate	18194115	1
Caesar & Loretz GmbH/Gehe	Prednicarbate	191226	1
Caesar & Loretz GmbH/GEHE	Prednicarbate	19122602	1
Caesar & Loretz GmbH/Gehe	Prednicarbate	19122604	1
Caesar & Loretz GmbH/Gehe	Prednicarbate	20000609004	1
Caesar & Loretz GmbH/Gehe	Prednicarbate	20000609006	1
Caesar & Loretz GmbH/Gehe	Prednicarbate	20000609009	1
Caesar & Loretz GmbH/Gehe	Prednicarbate	21000991003	1
Caesar & Loretz GmbH/Gehe	Prednicarbate	21001161006	1
Caesar & Loretz GmbH...	Prednicarbate	21000991002	1
Caesar & Loretz GmbH...	Prednicarbate	21001161006	1
Caesar & Loretz GmbH...	Prednicarbate	18194117	1
Caesar & Loretz GmbH...	Prednicarbate	20003660009	1
Caesar & Loretz GmbH...	Prednicarbate	21001161006	2
Caesar & Loretz GmbH...	Prednicarbate	19122604	1
Caesar & Loretz GmbH...	Prednicarbate	20000609004	1
Caesar & Loretz GmbH...	Prednicarbate	20003660004	1
Caesar & Loretz GmbH...	Prednicarbate	21001161007	1
Caesar & Loretz GmbH...	Prednicarbate	21001161011	1
Caesar & Loretz GmbH...	Prednicarbate	19051602	1
Caesar & Loretz GmbH...	Prednicarbate	20003660005	1
Caesar & Loretz GmbH...	Prednicarbate	21000991002	1
Caesar & Loretz GmbH...	Prednicarbate	21001161001	6
Caesar & Loretz GmbH...	Prednicarbate	21001161006	1
Caesar & Loretz GmbH...	Prednicarbate	19122602	1
Caesar & Loretz GmbH...	Prednicarbate	20000609009	1
Caesar & Loretz GmbH...	Prednicarbate	20003660008	1
Caesar & Loretz GmbH/sa	Prednicarbate	22000755001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Prednicarbate	19122604	1
Caesar & Loretz GmbH...	Prednicarbate	20003660007	1
Caesar & Loretz GmbH...	Prednicarbate	21001161001	1
Caesar & Loretz GmbH...	Prednicarbate	AP221018-02	1
Caesar & Loretz GmbH	Prednicarbate	16087410	1
Caesar & Loretz GmbH	Prednicarbate	18194103	1
Caesar & Loretz GmbH	Prednicarbate	18194104	1
Caesar & Loretz GmbH	Prednicarbate	18194105	12
Caesar & Loretz GmbH	Prednicarbate	18194115	10
Caesar & Loretz GmbH	Prednicarbate	18194117	1
Caesar & Loretz GmbH	Prednicarbate	19051601	1
Caesar & Loretz GmbH	Prednicarbate	19051602	10
Caesar & Loretz GmbH	Prednicarbate	19122602	4
Caesar & Loretz GmbH	Prednicarbate	19122604	6
Caesar & Loretz GmbH	Prednicarbate	19122608	7
Caesar & Loretz GmbH	Prednicarbate	20000609004	16
Caesar & Loretz GmbH	Prednicarbate	20000609006	6
Caesar & Loretz GmbH	Prednicarbate	20000609009	14
Caesar & Loretz GmbH	Prednicarbate	20003660004	5
Caesar & Loretz GmbH	Prednicarbate	20003660005	4
Caesar & Loretz GmbH	Prednicarbate	20003660006	5
Caesar & Loretz GmbH	Prednicarbate	20003660007	10
Caesar & Loretz GmbH	Prednicarbate	20003660008	13
Caesar & Loretz GmbH	Prednicarbate	20003660009	4
Caesar & Loretz GmbH	Prednicarbate	21000991002	8
Caesar & Loretz GmbH	Prednicarbate	21000991003	10
Caesar & Loretz GmbH	Prednicarbate	21000991005	8
Caesar & Loretz GmbH	Prednicarbate	21001161001	14
Caesar & Loretz GmbH	Prednicarbate	21001161004	3
Caesar & Loretz GmbH	Prednicarbate	21001161006	11
Caesar & Loretz GmbH	Prednicarbate	21001161007	10
Caesar & Loretz GmbH	Prednicarbate	21001161008	4
Caesar & Loretz GmbH	Prednicarbate	21001161010	6
Caesar & Loretz GmbH	Prednicarbate	21001161011	9
Caesar & Loretz GmbH	Prednicarbate	21001161013	2
Caesar & Loretz GmbH	Prednicarbate	21A11-B01-2035804	1
Caesar & Loretz GmbH	Prednicarbate	22000755001	5
Caesar & Loretz GmbH	Prednicarbate	22000755002	3
Caesar & Loretz GmbH	Prednicarbate	22000755003	6
Caesar & Loretz GmbH	Prednicarbate	22000755005	1
Caesar & Loretz GmbH	Prednicarbate	22000755007	7
Caesar & Loretz GmbH	Prednicarbate	22000755009	2
Caesar & Loretz GmbH	Prednicarbate	22000755010	1
Caesar & Loretz GmbH	Prednicarbate	23001026001	2
Caesar & Loretz GmbH	Prednicarbate	23001026002	1
Caesar & Loretz Hild...	Prednicarbate	19051602	2
Caesar & Loretz Hild...	Prednicarbate	20000609004	1
Caesar & Loretz Hilden	Prednicarbate	18194104	1
Caesar & Loretz Hilden	Prednicarbate	19122608	2
Caesar & Loretz Hilden	Prednicarbate	20000609009	2
Caesar & Loretz Hilden	Prednicarbate	2009018-01	1
Caesar & Loretz/Geil...	Prednicarbate	19051602	1
Caesar & Loretz/Noweda	Prednicarbate	20000609004	1
Caesar & Loretz/Noweda	Prednicarbate	20003660005	1
Caesar Loretz	Prednicarbate	20003660007	1
Caesar und Loretz GmbH	Prednicarbate	17220406	1
caesar&loretz GmbH,A...	Prednicarbate	16087408	1
Caesar&Loretz GmbH/ ...	Prednicarbate	19122604	1
Caesar&Loretz GmbH	Prednicarbate	20003660006	1
Caesar&Loretz GmbH	Prednicarbate	22000755003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
caesar&loretz,Phönix	Prednicarbate	15181411	1
caesar&loretz	Prednicarbate	18149103	1
Caesar/Ebert	Prednicarbate	18194105	1
Caleo/ Fiebig	Prednicarbate	17J04-B05-341872	1
Caleo/Krieger	Prednicarbate	21001161007	1
Cealo/GEHE	Prednicarbate	17315609	1
Cealo/Jenne	Prednicarbate	220306(21001161006)	1
Cealo/Phönix	Prednicarbate	20000609004	1
Cealo/Sanacorp	Prednicarbate	15546306	1
cealo	Prednicarbate	14J16-B06-303465	1
Celo	Prednicarbate	1687408	1
Defektur	Prednicarbate	12D27-N04	1
E und J, 22.07.2016	Prednicarbate	15446306	2
Eu Rho	Prednicarbate	2103017-01	1
Eurho / Alliance	Prednicarbate	2103017-01	2
EuRho / Noweda	Prednicarbate	1903023-01	4
EuRho/ AHD	Prednicarbate	1801013-01	1
EuRho/ AHD	Prednicarbate	1805005	1
EuRho/ NOWEDA	Prednicarbate	1903023-01	1
EuRho/ NOWEDA	Prednicarbate	2001031-01	1
EuRho/Gehe	Prednicarbate	1801013-01	2
eurho/gehe	Prednicarbate	2009018-01	1
EuRho/Noweda	Prednicarbate	1805005-01	1
EuRho/Noweda	Prednicarbate	200901801	1
Eurho/noweda	Prednicarbate	210301701	1
EuRho/Phoenix	Prednicarbate	2009018-01	1
EuRho/Phönix	Prednicarbate	1805005-01	2
EuRho/Phönix	Prednicarbate	2001031-01	1
EuRho	Prednicarbate	1801013-01	1
EuRho	Prednicarbate	2103017-01	1
Euro OCT / Krieger	Prednicarbate	2009018-01	6
Euro OTC	Prednicarbate		3
Euro OTC	Prednicarbate	1302033-01	1
Euro OTC	Prednicarbate	1302033-02	3
Euro OTC	Prednicarbate	13224402	1
Euro OTC	Prednicarbate	13372403	1
Euro OTC	Prednicarbate	1501033-01	2
Euro OTC	Prednicarbate	1501033-02	4
Euro OTC	Prednicarbate	1507011-01	2
Euro OTC	Prednicarbate	1507011-02	4
Euro OTC	Prednicarbate	1601058-01	5
Euro OTC	Prednicarbate	1605001	1
Euro OTC	Prednicarbate	1605001-01	10
Euro OTC	Prednicarbate	1607012-01	11
Euro OTC	Prednicarbate	1609011-01	1
Euro OTC	Prednicarbate	160902	1
Euro OTC	Prednicarbate	160902201	3
Euro OTC	Prednicarbate	1609022-01	21
Euro OTC	Prednicarbate	170702201	1
Euro OTC	Prednicarbate	1707022-01	40
Euro OTC	Prednicarbate	1707022201	1
Euro OTC	Prednicarbate	17220408	2
Euro OTC	Prednicarbate	1801013	1
Euro OTC	Prednicarbate	180101301	1
Euro OTC	Prednicarbate	1801013-01	33
Euro OTC	Prednicarbate	1805001-01	2
Euro OTC	Prednicarbate	180500501	1
Euro OTC	Prednicarbate	1805005-01	27
Euro OTC	Prednicarbate	1805005-02	2
Euro OTC	Prednicarbate	1809015001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Prednicarbate	180901501	4
Euro OTC	Prednicarbate	1809015-01	37
Euro OTC	Prednicarbate	1809015-02	2
Euro OTC	Prednicarbate	18E14-B03-355726	1
Euro OTC	Prednicarbate	190023-01	1
Euro OTC	Prednicarbate	1902012-01	1
Euro OTC	Prednicarbate	1903023	2
Euro OTC	Prednicarbate	190302301	3
Euro OTC	Prednicarbate	1903023-01	76
Euro OTC	Prednicarbate	1903023-02	1
Euro OTC	Prednicarbate	19032023-01	1
Euro OTC	Prednicarbate	190741607	1
Euro OTC	Prednicarbate	20001031-01	1
Euro OTC	Prednicarbate	20009018-01	1
Euro OTC	Prednicarbate	200103101	5
Euro OTC	Prednicarbate	2001031-01	83
Euro OTC	Prednicarbate	20090018-01	1
Euro OTC	Prednicarbate	200901-01	1
Euro OTC	Prednicarbate	200901801	3
Euro OTC	Prednicarbate	2009018-01	149
Euro OTC	Prednicarbate	2009018-012x	1
Euro OTC	Prednicarbate	2009018-02	22
Euro OTC	Prednicarbate	200918-01	2
Euro OTC	Prednicarbate	209018-01	1
Euro OTC	Prednicarbate	210301701	3
Euro OTC	Prednicarbate	2103017-01	68
Euro OTC	Prednicarbate	2103017-02	4
Euro OTC	Prednicarbate	210317-01	1
Euro OTC	Prednicarbate	2204014_01	1
Euro OTC	Prednicarbate	2204014-01	16
Euro OTC	Prednicarbate	220414-01	1
Euro OTC	Prednicarbate	23001026001	1
Euro OTC	Prednicarbate	2304020-01	1
Euro OTC	Prednicarbate	3103017-01	1
Euro OTC	Prednicarbate	B01-2035804	1
Euro OTC	Prednicarbate	B05-2016409	1
Euro OTC	Prednicarbate	PNC101/0720	1
Euro Pharma/Gehe	Prednicarbate	1801013-01	1
Euro/Gehe	Prednicarbate	1609022-01	1
Euro/Gehe	Prednicarbate	1805005-01	1
Euro/Phönix	Prednicarbate	1607012-01	1
Euro/Phönix	Prednicarbate	1809015-01	2
Euro/Phönix	Prednicarbate	1903023-01	1
Euro/Phönix	Prednicarbate	2204014-01	1
Euro	Prednicarbate	1507011-01	1
EuRoh/ Gehe	Prednicarbate	18E14-B03-355726	2
Fagr	Prednicarbate	18E14-B03-352560	2
Fagro/Gehe	Prednicarbate	15D15-B03-308161	1
Fagro/Sanacorp	Prednicarbate	19G09-B01-194724	1
Fagron	Prednicarbate		1
Fagron	Prednicarbate	10J04-N10	1
Fagron	Prednicarbate	11L23-N07	4
Fagron	Prednicarbate	12B20-N06	3
Fagron	Prednicarbate	12D27-N04	3
Fagron	Prednicarbate	12H20-N07	1
Fagron	Prednicarbate	13/23-N04	3
Fagron	Prednicarbate	13372408	1
Fagron	Prednicarbate	13C25-N02	1
Fagron	Prednicarbate	13C25-N06	7
Fagron	Prednicarbate	13c25-no6	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednicarbate	13F11-N01	4
Fagron	Prednicarbate	13F11-No1	1
Fagron	Prednicarbate	13F11-NO1	1
Fagron	Prednicarbate	13G05-N03	5
Fagron	Prednicarbate	13I23-N04	8
Fagron	Prednicarbate	13l23-N04	1
Fagron	Prednicarbate	14A27-B02	2
Fagron	Prednicarbate	14a27-b02-291256	2
Fagron	Prednicarbate	14A27-B02-291256	17
Fagron	Prednicarbate	14A27-B02-291258	2
Fagron	Prednicarbate	14A27-B02-295793	1
Fagron	Prednicarbate	14A27-B02-295796	6
Fagron	Prednicarbate	14A27-B02-295797	7
Fagron	Prednicarbate	14B13-B31-291255	1
Fagron	Prednicarbate	14J16B06	1
Fagron	Prednicarbate	14J16-B06_303465	1
Fagron	Prednicarbate	14J16-B06-303465	14
Fagron	Prednicarbate	14J16B06303466	1
Fagron	Prednicarbate	15/22-B04-316799	1
Fagron	Prednicarbate	15D15-B03-30816	1
Fagron	Prednicarbate	15D15-B03308161	1
Fagron	Prednicarbate	15D15-B03-308161	9
Fagron	Prednicarbate	15D15-B03-308162	1
Fagron	Prednicarbate	15D15-B03-309682	1
Fagron	Prednicarbate	15E14-B03-355726	1
Fagron	Prednicarbate	15G10-B02	1
Fagron	Prednicarbate	15g10-b02-310848	1
Fagron	Prednicarbate	15G10-B02-310848	9
Fagron	Prednicarbate	15G10-B02-311819	1
Fagron	Prednicarbate	15G10-B02-314082	4
Fagron	Prednicarbate	15J22-B04	1
Fagron	Prednicarbate	15J22-B04-316799	6
Fagron	Prednicarbate	15J22-B04-318528	3
Fagron	Prednicarbate	15J22-B04-318930	6
Fagron	Prednicarbate	15J22-B04-321005	1
Fagron	Prednicarbate	15J22-BO4-316799	1
Fagron	Prednicarbate	15J-B04-316799	1
Fagron	Prednicarbate	16/27B01-332958	1
Fagron	Prednicarbate	16/27-B01-332958	2
Fagron	Prednicarbate	160314PC	1
Fagron	Prednicarbate	160518P	1
Fagron	Prednicarbate	16087410	1
Fagron	Prednicarbate	160902201	1
Fagron	Prednicarbate	1612-B01-325758	1
Fagron	Prednicarbate	16A18/B01	1
Fagron	Prednicarbate	16A18-B01-322732	6
Fagron	Prednicarbate	16E12-B01	2
Fagron	Prednicarbate	16E12-B01-325758	6
Fagron	Prednicarbate	16E12-B01-327344	3
Fagron	Prednicarbate	16E12-B01-32827	1
Fagron	Prednicarbate	16E12-B01-328270	6
Fagron	Prednicarbate	16E12-B01-330093	2
Fagron	Prednicarbate	16G09-B01-194722	2
Fagron	Prednicarbate	16J27-B01	2
Fagron	Prednicarbate	16j27b01330976	1
Fagron	Prednicarbate	16j27-b01-330976	1
Fagron	Prednicarbate	16J27-b01-330976	1
Fagron	Prednicarbate	16J27-B01-330976	12
Fagron	Prednicarbate	16J27-B01-330977	1
Fagron	Prednicarbate	16J27-B01-332958	13

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednicarbate	16J28-B01-330976	1
Fagron	Prednicarbate	17013804	1
Fagron	Prednicarbate	17104-805-343934	1
Fagron	Prednicarbate	17220407	2
Fagron	Prednicarbate	174J04-B05-343935	1
Fagron	Prednicarbate	17C27-B01	1
Fagron	Prednicarbate	17C27-B01-335530	10
Fagron	Prednicarbate	17C27-B01-335531	1
Fagron	Prednicarbate	17c27-b01-339079	1
Fagron	Prednicarbate	17C27-B01-339079	8
Fagron	Prednicarbate	17J04-B05	4
Fagron	Prednicarbate	17J04-B05-326113	1
Fagron	Prednicarbate	17J04-B05-340570	2
Fagron	Prednicarbate	17J04-B05-341872	9
Fagron	Prednicarbate	17j04-b05-343934	1
Fagron	Prednicarbate	17J04-B05-343934	9
Fagron	Prednicarbate	17J04-B05-343935	1
Fagron	Prednicarbate	17J04b05-346113	1
Fagron	Prednicarbate	17J04-B05-346113	10
Fagron	Prednicarbate	17Jo4B05343934	1
Fagron	Prednicarbate	1801013-01	4
Fagron	Prednicarbate	18194104	1
Fagron	Prednicarbate	18194105	1
Fagron	Prednicarbate	18194115	1
Fagron	Prednicarbate	18B17-B01-347486	1
Fagron	Prednicarbate	18B27-01-347486	1
Fagron	Prednicarbate	18B27-01-350264	1
Fagron	Prednicarbate	18B27-B01	2
Fagron	Prednicarbate	18B27-B01_347486	1
Fagron	Prednicarbate	18B27-B01-0001	1
Fagron	Prednicarbate	18B27-B01-346748	2
Fagron	Prednicarbate	18B27-B01-347486	20
Fagron	Prednicarbate	18B27-B01-350264	12
Fagron	Prednicarbate	18B27-B01-351177	3
Fagron	Prednicarbate	18E14-03-352631	1
Fagron	Prednicarbate	18E14-B03	5
Fagron	Prednicarbate	18E14B03-352560	1
Fagron	Prednicarbate	18E14-B03-352560	7
Fagron	Prednicarbate	18E14-B03-35260	1
Fagron	Prednicarbate	18E14-B03-352631	10
Fagron	Prednicarbate	18e14-b03-355726	1
Fagron	Prednicarbate	18E14-B03-355726	11
Fagron	Prednicarbate	18E-14-B03-355726	1
Fagron	Prednicarbate	18E14-B03-355727	3
Fagron	Prednicarbate	18J27-B01-332958	1
Fagron	Prednicarbate	194722	1
Fagron	Prednicarbate	19E14	1
Fagron	Prednicarbate	19E14-B01	1
Fagron	Prednicarbate	19E14-B01-191430	19
Fagron	Prednicarbate	19E14-B01-191431	3
Fagron	Prednicarbate	19G09-B01	3
Fagron	Prednicarbate	19G09-B01-194722	17
Fagron	Prednicarbate	19G09-B01-194724	3
Fagron	Prednicarbate	19J16-B04-197550	1
Fagron	Prednicarbate	19J16-B07	6
Fagron	Prednicarbate	19J16B07197550	1
Fagron	Prednicarbate	19J16-B07197550	1
Fagron	Prednicarbate	19J16-B07-197550	15
Fagron	Prednicarbate	19J16-B07-197552	3
Fagron	Prednicarbate	19J16-B07-197555	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednicarbate	19J16-B07-20137002	1
Fagron	Prednicarbate	19J16-B07-201371	1
Fagron	Prednicarbate	19J16-B07-201372	15
Fagron	Prednicarbate	19J16-BO7-197550	1
Fagron	Prednicarbate	19J16-BO7-197552	1
Fagron	Prednicarbate	19J16-BO7-201372	1
Fagron	Prednicarbate	19J19-B07-197550	1
Fagron	Prednicarbate	20/18-B05-201649	1
Fagron	Prednicarbate	20003660007	1
Fagron	Prednicarbate	2001031-01	1
Fagron	Prednicarbate	20A21-B12	8
Fagron	Prednicarbate	20A21-B12-196767	1
Fagron	Prednicarbate	20A21-B12-1975501	2
Fagron	Prednicarbate	20A21-B12-197551	9
Fagron	Prednicarbate	20A21-B12-197553	3
Fagron	Prednicarbate	20A21-B12-197556	1
Fagron	Prednicarbate	20G23-B06	1
Fagron	Prednicarbate	20G23-B06-200074	1
Fagron	Prednicarbate	20g23-b06-200202	1
Fagron	Prednicarbate	20G23-B06-200202	2
Fagron	Prednicarbate	20I18-B05	3
Fagron	Prednicarbate	20I18-B05-2016409	1
Fagron	Prednicarbate	20I18-B05-201649	10
Fagron	Prednicarbate	20I8-B05-201649	1
Fagron	Prednicarbate	21a11-801-203584	1
Fagron	Prednicarbate	21A11-B01	6
Fagron	Prednicarbate	21A11-B01-201650	11
Fagron	Prednicarbate	21A11-B01-201651	1
Fagron	Prednicarbate	21A11-B01-2035804	2
Fagron	Prednicarbate	21A11B01203584	1
Fagron	Prednicarbate	21A11-B01-203584	31
Fagron	Prednicarbate	21A11-BO1-203584	1
Fagron	Prednicarbate	21F07-B17	1
Fagron	Prednicarbate	21F07-B17-216553	43
Fagron	Prednicarbate	21-F07-B17-216553	1
Fagron	Prednicarbate	21F07-B17-216554	3
Fagron	Prednicarbate	21FO7-0001	1
Fagron	Prednicarbate	21FO7-B17-216553	1
Fagron	Prednicarbate	21K24-B03-213700	2
Fagron	Prednicarbate	21K24-Bo3-213700	1
Fagron	Prednicarbate	22F03-B02-223102	2
Fagron	Prednicarbate	22F03-B02-227918	2
Fagron	Prednicarbate	22F03-B02-227919	1
Fagron	Prednicarbate	2762	1
Fagron	Prednicarbate	29091807	1
Fagron	Prednicarbate	2OG23-BO6-200074	1
Fagron	Prednicarbate	3251	1
Fagron	Prednicarbate	4111706	1
Fagron	Prednicarbate	701867	1
Fagron	Prednicarbate	701867-0001	2
Fagron	Prednicarbate	7061303	1
Fagron	Prednicarbate	8081403	1
Fagron	Prednicarbate	9E04-N02	1
Fagron	Prednicarbate	9G14-N06	1
Fagron	Prednicarbate	B01-2016500	1
Fagron	Prednicarbate	b01-2035804	1
Fagron	Prednicarbate	B01-2035804	9
Fagron	Prednicarbate	B01-203584	1
Fagron	Prednicarbate	B03-3557206	1
Fagron	Prednicarbate	B05-2016409	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednicarbate	B06-2002002	1
Fagron	Prednicarbate	B07-2013702	1
Fagron	Prednicarbate	B12-1975501	5
Fagron	Prednicarbate	B01-2035804	1
Fagron	Prednicarbate	htzthh	1
Fagron	Prednicarbate	na1668m	1
Fagron	Prednicarbate	NA2374M	2
Fagron	Prednicarbate	NT0555M13I23-N04	1
Fagron	Prednicarbate	NT0780M	2
Fagron	Prednicarbate	NU0823M	1
Fagron	Prednicarbate	NUO823M	1
Fagron	Prednicarbate	NV2209M	1
Fagron	Prednicarbate	NW0396M	1
Fagron	Prednicarbate	NX1422M	3
Fagron	Prednicarbate	NX1925M	3
Fagron	Prednicarbate	NX2297M	6
Fagron	Prednicarbate	NZ1045M	5
Fagron	Prednicarbate	PNC102/1020	6
Fargon / AHD	Prednicarbate	21A11-B01-203584	1
Fargon/Phoenix 05.06.18	Prednicarbate	17J04-B05-343934	1
Fargon/Phönix	Prednicarbate	19J16-B07	1
Fargon	Prednicarbate	15J22-B04-318930	1
Fargon	Prednicarbate	16E12-B01_325758	1
Fargon	Prednicarbate	19G09-B01	1
Fargon	Prednicarbate	21A11-B01-203584	2
Farmabios S.p.A.	Prednicarbate	20003660009	1
Farmabios S.p.A/AHD	Prednicarbate	20000609006	1
Fiebig Palapharm	Prednicarbate	20000609004	1
Fiebig	Prednicarbate	17013804	1
Fiebig	Prednicarbate	17220408	1
Fiebig	Prednicarbate	18194105	1
Fiebig	Prednicarbate	20003660009	1
Fischar/ Noweda	Prednicarbate	21F07-B17-216553	1
Fragon/Sanacorp	Prednicarbate	NZ1845M	1
Fragron	Prednicarbate	NV0485M	1
Gehe amax	Prednicarbate	1507011-01	1
Gehe amax	Prednicarbate	15G10-B02-314082	1
Gehe amax	Prednicarbate	15J22-B04-316799	1
Gehe amax	Prednicarbate	1607012-01	1
Gehe amax	Prednicarbate	16J27-B01-330976	1
Gehe amax	Prednicarbate	1707022-01	2
Gehe amax	Prednicarbate	18B27-B01-350264	1
Gehe amax	Prednicarbate	20003660005	1
Gehe Rostock	Prednicarbate	19J16-B07-197550	1
Gehe Rostock	Prednicarbate	19J16-B07-201372	1
Gehe	Prednicarbate	12B14-N02	1
Gehe	Prednicarbate	13G05-n03	1
Gehe	Prednicarbate	13123-N04	1
Gehe	Prednicarbate	15446302	1
Gehe	Prednicarbate	15J22-B04-318930	1
Gehe	Prednicarbate	15J22-B04-321005	1
Gehe	Prednicarbate	1601058-01	1
Gehe	Prednicarbate	1605001-01	2
Gehe	Prednicarbate	1707022-01	3
GEHE	Prednicarbate	17315607	2
Gehe	Prednicarbate	1801013-01	5
Gehe	Prednicarbate	1805005-01	1
Gehe	Prednicarbate	1809015-01	4
GEHE	Prednicarbate	18194103	4
Gehe	Prednicarbate	18194105	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
GEHE	Prednicarbate	18194116	1
Gehe	Prednicarbate	18E14-B03	1
Gehe	Prednicarbate	1903023-01	3
Gehe	Prednicarbate	19032301	1
Gehe	Prednicarbate	19051601	1
Gehe	Prednicarbate	19122604	2
Gehe	Prednicarbate	19G09-B01	1
Gehe	Prednicarbate	19G09-B01-194722	2
Gehe	Prednicarbate	19J16-B07	1
Gehe	Prednicarbate	20003660004	1
Gehe	Prednicarbate	2009018-01	2
Gehe	Prednicarbate	20G23-B06	2
Gehe	Prednicarbate	21000991005	3
Gehe	Prednicarbate	21001161001	2
Gehe	Prednicarbate	21001161011	1
Gehe	Prednicarbate	21A11-B01	3
Gehe	Prednicarbate	21F07-B17	1
Gehe	Prednicarbate	21F07-B17-216553	1
Gehe	Prednicarbate	22000755002	2
Gehe	Prednicarbate	22000755007	1
Gehe	Prednicarbate	2204014-01	1
Gehe	Prednicarbate	22F03-B02-227918	1
Gehe	Prednicarbate	23001026001	5
Gehe	Prednicarbate	23001026002	2
Gehe	Prednicarbate	2304020-01	1
Gehe	Prednicarbate	2OG23-BO6-200202	1
GEHE	Prednicarbate	7529666	1
Gehe	Prednicarbate	B01-2016500	1
Gehe	Prednicarbate	C0333/1170101	1
Hedinger/ Sanacorp	Prednicarbate	15181403	1
Hedinger	Prednicarbate	16J27-B01-330976	2
Henry Lamotte	Prednicarbate	15D15-B03-308161	1
Hepart	Prednicarbate	17C27-B01-335530	1
JENNE	Prednicarbate	17220406	2
JENNE	Prednicarbate	17315603	1
Jenne	Prednicarbate	17J04-B05-346113	1
Jenne	Prednicarbate	18194105	1
Jenne	Prednicarbate	18194115	2
Jenne	Prednicarbate	1903023-01	1
Jenne	Prednicarbate	19J16-B07-197552	1
JENNE	Prednicarbate	22000755009	1
Jenne	Prednicarbate	23001026001	2
Jenne	Prednicarbate	P2019/91	1
Kehr Holdermann	Prednicarbate	23001026003	1
Kehr/Fargon	Prednicarbate	17J04-B05-346113	1
Kehr/Fargon	Prednicarbate	18B27-B01-350264	2
Kehr	Prednicarbate	16J27-B01-330976	1
Kehr	Prednicarbate	22000755006	1
Kehr	Prednicarbate	22000755010	3
Kehr	Prednicarbate	23001026001	4
Kehr	Prednicarbate	23001026002	1
Klenk	Prednicarbate	17014003	1
Krieger	Prednicarbate	2009018-01	1
Kriegeram 29.06.2018	Prednicarbate	17315605	1
Newchem / Gehe	Prednicarbate	18E14-B03-355726	1
Newchem / Gehe	Prednicarbate	19E14-B01-191430	1
Newchem / Gehe	Prednicarbate	B07-2013702	1
Newchem spa/Noweda	Prednicarbate	14A27-B02-291256	1
Newchem Spa/Sanacorp	Prednicarbate	16E12-B01	1
Newchem/ AHD	Prednicarbate	19122602	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Newchem/Phoenix	Prednicarbate	20I18-B05	1
NEWCHEM	Prednicarbate	19E14-B01-191430	2
Noveda	Prednicarbate	21A11-B01-203584	1
Noweda 17.11.17	Prednicarbate	17220407	1
Noweda Taucha	Prednicarbate	21001161010	1
Noweda	Prednicarbate	15446301	1
Noweda	Prednicarbate	161001	1
Noweda	Prednicarbate	17013804	2
Noweda	Prednicarbate	17315604	1
Noweda	Prednicarbate	17315605	1
Noweda	Prednicarbate	17315609	1
Noweda	Prednicarbate	17J04-B05-346113	1
Noweda	Prednicarbate	1801013-01	1
Noweda	Prednicarbate	1805005-01	1
Noweda	Prednicarbate	19122608	1
Noweda	Prednicarbate	20000366007	1
Noweda	Prednicarbate	20003660007	1
Noweda	Prednicarbate	21001161001	1
Noweda	Prednicarbate	2103017-01	4
Noweda	Prednicarbate	211867001	1
Noweda	Prednicarbate	21a11b01203584no	1
Noweda	Prednicarbate	21F07b17	1
Noweda	Prednicarbate	21K24-B03-2136699	1
Noweda	Prednicarbate	21K24-B03-213699	2
Noweda	Prednicarbate	22000755001	1
Noweda	Prednicarbate	2200755007	1
Noweda	Prednicarbate	2204014-01	1
Noweda	Prednicarbate	22F03-B02-223102	1
Noweda	Prednicarbate	22F03-B02-227918	1
Noweda	Prednicarbate	22F03-B02-227919	1
Noweda	Prednicarbate	23001025003	2
Noweda	Prednicarbate	23001026001	4
noweda	Prednicarbate	231001026003	1
Nowerda	Prednicarbate	17J04-B05-343934	1
Nowerda	Prednicarbate	18B27-B01-347486	1
Nowerda	Prednicarbate	18E14-B03-352560	1
Ph Eur/Ph	Prednicarbate	2103017-01	3
Phoenix 7.02.2020	Prednicarbate	1903023-01	1
phoenix	Prednicarbate	1323N04	1
Phoenix	Prednicarbate	16J27-b01-332958	1
Phoenix	Prednicarbate	17315604	3
Phoenix	Prednicarbate	17315605	1
Phoenix	Prednicarbate	17C27-B01-335530	1
Phoenix	Prednicarbate	1903023-02	1
Phoenix	Prednicarbate	19122602	1
Phoenix	Prednicarbate	20000609009	2
Phoenix	Prednicarbate	20003660007	1
Phoenix	Prednicarbate	22000755010	1
Phoenix	Prednicarbate	23001025003	1
Phoenix	Prednicarbate	23001026002	3
Phoenix	Prednicarbate	3070	1
Phoenix	Prednicarbate	3089	1
Phoenix	Prednicarbate	3097	1
Phoenix	Prednicarbate	3106	1
Phoenix	Prednicarbate	3119	1
Phoenix	Prednicarbate	3208	1
Phoenix	Prednicarbate	3239	1
Phoenix	Prednicarbate	3363	1
Phoenix	Prednicarbate	3408	1
Phoenix	Prednicarbate	B05-2016409	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix Gotha	Prednicarbate	17220408	1
Phönix	Prednicarbate	15J22-B04-318528	1
Phönix	Prednicarbate	16J27-B01-330976	1
Phönix	Prednicarbate	1707022-01	1
Phönix	Prednicarbate	18194104	2
Phönix	Prednicarbate	1903023-01	1
PHÖNIX	Prednicarbate	1903023-01	1
Phönix	Prednicarbate	20003660007	2
Phönix	Prednicarbate	2001031-01	4
Phönix	Prednicarbate	2009018-01	1
Phönix	Prednicarbate	20D07-F01370645	1
PHÖNIX	Prednicarbate	21001161001	1
Phönix	Prednicarbate	210301701	1
Phönix	Prednicarbate	2103017-01	2
phönix	Prednicarbate	21F07-B17-216553	1
Phönix	Prednicarbate	2204014-01	1
phönix	Prednicarbate	22F03-B02-223102	1
Phönix	Prednicarbate	22F03-B02-223102	1
Phönix	Prednicarbate	23001025003	1
Phönix	Prednicarbate	23001026002	2
Phönix	Prednicarbate	23003318006	1
Phönix	Prednicarbate	3134	1
Phönix	Prednicarbate	3154	1
Phönix	Prednicarbate	3185	1
Sanacop	Prednicarbate		3
Sanacorp, 01.03.17, …	Prednicarbate	1687410	1
Sanacorp	Prednicarbate	11L23-N07	1
Sanacorp	Prednicarbate	17013804	1
Sanacorp	Prednicarbate	1707022-01	1
Sanacorp	Prednicarbate	17315604	2
Sanacorp	Prednicarbate	17315605	1
Sanacorp	Prednicarbate	18194105	1
Sanacorp	Prednicarbate	18194115	1
sanacorp	Prednicarbate	1903023-01	1
Sanacorp	Prednicarbate	20000609009	1
Sanacorp	Prednicarbate	20A-21-B12-197551	1
Sanacorp	Prednicarbate	20A21-B12-197553	1
Sanacorp	Prednicarbate	22000755009	2
Sanacorp	Prednicarbate	22F03-B02-223103	1
Sanacorp	Prednicarbate	23001026001	1
Sanacorp	Prednicarbate	B05-2016409	1
Sino Phyto	Prednicarbate	13224401	1
Sonnenberg-Apotheke	Prednicarbate	1607012-01	1
Symbiotica	Prednicarbate	2103017-01	1
Symbiotika	Prednicarbate	2009018-01	1

- 232 088 spectra from 1515 *Apo-Ident* customers from a total of 48 748 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Prednicarbate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prednicarbate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	964	0	151 998
Type B	0	1297	0	200 787
Type C	0	3967	12	232 088

The substance/substance group *Prednicarbate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.3776 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.5374 %)
Type C	100.0000 % (> 99.9007 %)	99.6984 % (> 99.6230 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20700	21572	30.21	205.06
20832	20832	0.00	187.59
20833	20832	2.37	186.73
21368	21368	0.00	155.13
21369	21368	2.82	155.56
21572	21572	0.00	202.31
21610	21610	0.00	165.51
21858	21858	0.00	194.33
22366	22366	0.00	147.83
25119	25119	0.00	213.53
25401	25401	0.00	211.09
25609	25609	0.00	211.19
26084	26084	0.00	206.15
26393	26084	23.79	202.59
27277	27277	0.00	212.13

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical

variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Prednisolon dihydrogen phosphate dinatrium**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20212-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Prednisolon dihydrogen phosphate dinatrium; Prednisoloni natrii phosphas

Special notes

When selecting the *Prednisolon dihydrogen phosphate dinatrium* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Prednisolon dihydrogen phosphate dinatrium	9	3	117

Second-stage model

For differentiation of the substance/substance group *Prednisolon dihydrogen phosphate dinatrium* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Prednisolon dihydrogen phosphate dinatrium* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	66.63	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Prednisolon dihydrogen phosphate dinatrium* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Prednisolon dihydrogen phosphate dinatrium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Prednisolon dihydrogen ph…	13304703	20923	40	20130904
Caelo	Prednisolon dihydrogen ph…	13304704	21412	60	1411052
Caelo	Prednisolon dihydrogen ph…	16174715	23271	40	20160930
Caelo	Prednisolon dihydrogen ph…	20002455003	25393	40	20200824
Caelo	Prednisolon dihydrogen ph…	20002455003	25393SI	40	20200824
Fagron	Prednisolon dihydrogen ph…	14E07-B06-295251	21571	60	20140623
Fagron	Prednisolon dihydrogen ph…	18D23-B08-351348	24293	40	1812421
Fagron	Prednisolon dihydrogen ph…	18K27-B04-363613	25375	40	20190828
Fagron	Prednisolon dihydrogen ph…	21E25-F03-378586	25912	40	2204384
Fagron	Prednisolon dihydrogen ph…	21E25-F03-378586	25912SI	30	2204384
Fagron	Prednisolon dihydrogen ph…	24A29-B02-233778	27175	40	20240219
Fagron	Prednisolon dihydrogen ph…	24A29-B02-233778	27175SI	40	20240219

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 510 spectra of 12 reference samples from the substance/substance group *Prednisolon dihydrogen phosphate dinatrium*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 452 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 5 reference samples from the substance/substance group *Prednisolon dihydrogen phosphate dinatrium*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Prednisolon dihydrogen ph…	181940	24905	40
Caelo	Prednisolon dihydrogen ph…	21003179007	25987	40
Fagron	Prednisolon dihydrogen ph…	16I14-B03-328918	23270	40
Caelo	Prednisolon dihydrogen ph…	21003179007	25987SI	40
Fagron	Prednisolon dihydrogen ph…	18K27-B04-363613	25375SI†	40

- 201 884 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 294 spectra from 119 *Apo-Ident* customers from 125 batches from the substance/substance group *Prednisolon dihydrogen phosphate dinatrium*.

- Among them are spectra of independent samples from 117 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Prednisolon dihydrogen ph…	21E25-F03-378592	5
	Prednisolon dihydrogen ph…	21K16-B16-226142	3
	Prednisolon dihydrogen ph…	23001195003	1
	Prednisolon dihydrogen ph…	23001195004	1
	Prednisolon dihydrogen ph…	23003063002	1
	Prednisolon dihydrogen ph…	23003063003	1
	Prednisolon dihydrogen ph…	24A29-B02-233778	1
Alte Apotheke	Prednisolon dihydrogen ph…	15K27B09-318738	1
Caelo	Prednisolon dihydrogen ph…	14196602	1
Caelo	Prednisolon dihydrogen ph…	14E07-B06-295251	3
Caelo	Prednisolon dihydrogen ph…	15199602	2
Caelo	Prednisolon dihydrogen ph…	15199603	1
Caelo	Prednisolon dihydrogen ph…	16174701	1
Caelo	Prednisolon dihydrogen ph…	16174702	1
Caelo	Prednisolon dihydrogen ph…	16174706	1
Caelo	Prednisolon dihydrogen ph…	16174710	1
Caelo	Prednisolon dihydrogen ph…	17077502	2
Caelo	Prednisolon dihydrogen ph…	17077503	1
Caelo	Prednisolon dihydrogen ph…	17077508	2
Caelo	Prednisolon dihydrogen ph…	18024602	1
Caelo	Prednisolon dihydrogen ph…	18024604	2
Caelo	Prednisolon dihydrogen ph…	18194001	2
Caelo	Prednisolon dihydrogen ph…	18194002	6
Caelo	Prednisolon dihydrogen ph…	18194003	3
Caelo	Prednisolon dihydrogen ph…	18194006	9
Caelo	Prednisolon dihydrogen ph…	18194007	2
Caelo	Prednisolon dihydrogen ph…	18194010	1
Caelo	Prednisolon dihydrogen ph…	18194011	2
Caelo	Prednisolon dihydrogen ph…	19129302	2
Caelo	Prednisolon dihydrogen ph…	19129304	8
Caelo	Prednisolon dihydrogen ph…	19129306	4
Caelo	Prednisolon dihydrogen ph…	192754002	2
Caelo	Prednisolon dihydrogen ph…	19275402	2
Caelo	Prednisolon dihydrogen ph…	19275403	3
Caelo	Prednisolon dihydrogen ph…	20001707001	2
Caelo	Prednisolon dihydrogen ph…	20001707002	2
Caelo	Prednisolon dihydrogen ph…	20001707003	2
Caelo	Prednisolon dihydrogen ph…	20001707008	2
Caelo	Prednisolon dihydrogen ph…	20002455002	3
Caelo	Prednisolon dihydrogen ph…	20002455003	1
Caelo	Prednisolon dihydrogen ph…	20003761001	1
Caelo	Prednisolon dihydrogen ph…	20003761002	4
Caelo	Prednisolon dihydrogen ph…	20003761003	1
Caelo	Prednisolon dihydrogen ph…	2001707001	1
Caelo	Prednisolon dihydrogen ph…	21000431001	1
Caelo	Prednisolon dihydrogen ph…	21000431002	2
Caelo	Prednisolon dihydrogen ph…	21000431003	1
Caelo	Prednisolon dihydrogen ph…	21000431006	1
Caelo	Prednisolon dihydrogen ph…	21001330002	2
Caelo	Prednisolon dihydrogen ph…	21001330003	1
Caelo	Prednisolon dihydrogen ph…	2100317009	1
Caelo	Prednisolon dihydrogen ph…	21003179002	2
Caelo	Prednisolon dihydrogen ph…	21003179003	2
Caelo	Prednisolon dihydrogen ph…	21003179004	4
Caelo	Prednisolon dihydrogen ph…	21003179007	1
Caelo	Prednisolon dihydrogen ph…	21003179008	4
Caelo	Prednisolon dihydrogen ph…	21003179009	3
Caelo	Prednisolon dihydrogen ph…	22000048001	2
Caelo	Prednisolon dihydrogen ph…	22000048005	1
Caelo	Prednisolon dihydrogen ph…	2200048002	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednisolon dihydrogen ph…	2200048003	1
Caelo	Prednisolon dihydrogen ph…	23001195001	1
Caesar & Loretz GmbH…	Prednisolon dihydrogen ph…	19129302	1
Caesar & Loretz GmbH…	Prednisolon dihydrogen ph…	19275402	1
Caesar & Loretz GmbH…	Prednisolon dihydrogen ph…	19129306	1
Caesar & Loretz GmbH/Gehe	Prednisolon dihydrogen ph…	22000048003	1
Caesar & Loretz GmbH…	Prednisolon dihydrogen ph…	21000431001	2
Caesar & Loretz GmbH…	Prednisolon dihydrogen ph…	21003179004	1
Caesar & Loretz GmbH…	Prednisolon dihydrogen ph…	21000431001	2
Caesar & Loretz GmbH…	Prednisolon dihydrogen ph…	21003179004	1
Caesar & Loretz GmbH…	Prednisolon dihydrogen ph…	22000048003	1
Caesar & Loretz GmbH	Prednisolon dihydrogen ph…	18194006	1
Caesar & Loretz GmbH	Prednisolon dihydrogen ph…	19129302	1
Caesar & Loretz GmbH	Prednisolon dihydrogen ph…	19129304	4
Caesar & Loretz GmbH	Prednisolon dihydrogen ph…	19275402	2
Caesar & Loretz GmbH	Prednisolon dihydrogen ph…	19275403	1
Caesar & Loretz GmbH	Prednisolon dihydrogen ph…	20001707002	1
Caesar & Loretz GmbH	Prednisolon dihydrogen ph…	20002455002	1
Caesar & Loretz GmbH	Prednisolon dihydrogen ph…	20003761002	1
Caesar & Loretz GmbH	Prednisolon dihydrogen ph…	21000431001	2
Caesar & Loretz GmbH	Prednisolon dihydrogen ph…	21000431002	1
Caesar & Loretz GmbH	Prednisolon dihydrogen ph…	21000431006	1
Caesar & Loretz GmbH	Prednisolon dihydrogen ph…	21003179003	1
Caesar & Loretz GmbH	Prednisolon dihydrogen ph…	21003179007	1
Caesar & Loretz GmbH	Prednisolon dihydrogen ph…	21003179008	1
Caesar & Loretz GmbH	Prednisolon dihydrogen ph…	22000048002	1
Caesar & Loretz GmbH	Prednisolon dihydrogen ph…	22000048003	2
Caesar & Loretz/Gehe…	Prednisolon dihydrogen ph…	20001707001	1
Caesar & Loretz/Gehe	Prednisolon dihydrogen ph…	18194001	1
Fagron	Prednisolon dihydrogen ph…	11C18-N11	1
Fagron	Prednisolon dihydrogen ph…	11K11-N11	2
Fagron	Prednisolon dihydrogen ph…	12H30-N08	3
Fagron	Prednisolon dihydrogen ph…	13/27-N01	1
Fagron	Prednisolon dihydrogen ph…	13A10-N04	3
Fagron	Prednisolon dihydrogen ph…	13C26N06	1
Fagron	Prednisolon dihydrogen ph…	13H19N04	1
Fagron	Prednisolon dihydrogen ph…	13I27-N01	4
Fagron	Prednisolon dihydrogen ph…	14E07-B06-295251	1
Fagron	Prednisolon dihydrogen ph…	14E07-B06-295253	1
Fagron	Prednisolon dihydrogen ph…	14G30-B09	1
Fagron	Prednisolon dihydrogen ph…	14G30-B09-303012	7
Fagron	Prednisolon dihydrogen ph…	14g30-b09-303014	1
Fagron	Prednisolon dihydrogen ph…	14G30-B09-303014	4
Fagron	Prednisolon dihydrogen ph…	15f29-b11-309694	1
Fagron	Prednisolon dihydrogen ph…	15F29-B11-309694	1
Fagron	Prednisolon dihydrogen ph…	15J01-B02	4
Fagron	Prednisolon dihydrogen ph…	15J01-B02-312722	5
Fagron	Prednisolon dihydrogen ph…	15J01-B02-313610	3
Fagron	Prednisolon dihydrogen ph…	15J01-B02-317180	2
Fagron	Prednisolon dihydrogen ph…	15K27-B09	4
Fagron	Prednisolon dihydrogen ph…	15k27-b09-318738	1
Fagron	Prednisolon dihydrogen ph…	15K27-B09-318738	3
Fagron	Prednisolon dihydrogen ph…	15K27-B09-322162	1
Fagron	Prednisolon dihydrogen ph…	15K27-B09-322163	3
Fagron	Prednisolon dihydrogen ph…	15K27B09-326263	1
Fagron	Prednisolon dihydrogen ph…	15K27-B09-326263	3
Fagron	Prednisolon dihydrogen ph…	16/14-B03-328169	1
Fagron	Prednisolon dihydrogen ph…	16I14-B03	2
Fagron	Prednisolon dihydrogen ph…	16I14-B03-328169	2
Fagron	Prednisolon dihydrogen ph…	16I14-B03-328918	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednisolon dihydrogen ph…	17/27-b03-342560	1
Fagron	Prednisolon dihydrogen ph…	17/27-B03-345405	1
Fagron	Prednisolon dihydrogen ph…	17B08-B05	1
Fagron	Prednisolon dihydrogen ph…	17B08B05337466	1
Fagron	Prednisolon dihydrogen ph…	17B08-B05-337466	4
Fagron	Prednisolon dihydrogen ph…	17B08-B05-340336	2
Fagron	Prednisolon dihydrogen ph…	17I12-B03-354549	1
Fagron	Prednisolon dihydrogen ph…	17I27-B03	2
Fagron	Prednisolon dihydrogen ph…	17I27-B03-342560	1
Fagron	Prednisolon dihydrogen ph…	17I27-B03-344246	3
Fagron	Prednisolon dihydrogen ph…	17I27-B03-345405	1
Fagron	Prednisolon dihydrogen ph…	17I27-B03-348462	1
Fagron	Prednisolon dihydrogen ph…	17I27-B03-354549	2
Fagron	Prednisolon dihydrogen ph…	18B02-B04-352053	1
Fagron	Prednisolon dihydrogen ph…	18D23-B08-350207	1
Fagron	Prednisolon dihydrogen ph…	18D23-B08-351348	1
Fagron	Prednisolon dihydrogen ph…	18D23-B08-352211	1
Fagron	Prednisolon dihydrogen ph…	18K27-B04	2
Fagron	Prednisolon dihydrogen ph…	18K27-B04-363611	2
Fagron	Prednisolon dihydrogen ph…	18K27-B04-363613	1
Fagron	Prednisolon dihydrogen ph…	19118D23-B08-350207	1
Fagron	Prednisolon dihydrogen ph…	21E25-F03-378585	2
Fagron	Prednisolon dihydrogen ph…	21E25-F03-378591	1
Fagron	Prednisolon dihydrogen ph…	21K16-B16-226142	1
Fagron	Prednisolon dihydrogen ph…	NU1356	1
Fagron	Prednisolon dihydrogen ph…	PSP002/0816	2
Fagron	Prednisolon dihydrogen ph…	PSP004/0117	1
Gehe	Prednisolon dihydrogen ph…	22002348005	1
Newchem spa	Prednisolon dihydrogen ph…	15J01-B02-313610	2
Noweda	Prednisolon dihydrogen ph…	22002348005	1
Noweda	Prednisolon dihydrogen ph…	23001195002	1
Noweda	Prednisolon dihydrogen ph…	23001195003	2
Phoenix	Prednisolon dihydrogen ph…	192754004	1
Sanacorp	Prednisolon dihydrogen ph…	19129304	1
Sanacorp	Prednisolon dihydrogen ph…	21000431002	1
Sidonia	Prednisolon dihydrogen ph…	17I27-B03-342560	1
Sidonia	Prednisolon dihydrogen ph…	17I27-B03-344246	1
Sidonia	Prednisolon dihydrogen ph…	17I27-B03-345405	6
Symbiotica / Noweda	Prednisolon dihydrogen ph…	18K27-B04-3636101	1
Symbiotica / Noweda	Prednisolon dihydrogen ph…	B04-3636101	1

- 235 773 spectra from 1515 *Apo-Ident* customers from a total of 49 134 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Prednisolon dihydrogen phosphate dinatrium* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prednisolon dihydrogen phosphate dinatrium* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	510	0	152 452
Type B	0	200	0	201 884
Type C	0	291	3	235 773

The substance/substance group *Prednisolon dihydrogen phosphate dinatrium* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8235 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9007 %)	98.9796 % (> 97.9592 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20923	21412	17.14	153.54
21412	21412	0.00	147.00
21571	21412	21.11	143.37
23271	21412	14.96	160.79
24293	24293	0.00	130.92
25375	24293	78.53	152.65
25393	21412	13.94	148.06
25912	25912	0.00	163.42
27175	21412	50.77	164.53

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Prednisolone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20773-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Prednisolone; Prednisolonum

Special notes

When selecting the *Prednisolone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Prednisolone	14	11	453

Second-stage model

For differentiation of the substance/substance group *Prednisolone* the following second-stage model is used:

- Submodel 02

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Prednisolone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prednisolon dihydrogen phosphate di…	44.36	–
Polymyxin B sulfate	107.64	–
⋮	⋮	⋮
Methylprednisolone	>50	45.50
Triamcinolone acetonide	>50	67.78
Fluocinolone acetonide	>50	86.57
Betamethasone	>50	95.18
Dexamethasone	>50	96.60
Tyrothricin	>50	130.84
Gramicidin	>50	157.31

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Prednisolone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Prednisolone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Prednisolone	12324202	20773	40	20121113
Caelo	Prednisolone	12324226	21303	39	1411271
Caelo	Prednisolone	13343105	21449	60	1411232
Caelo	Prednisolone	154000	22435	60	20160225*
Caelo	Prednisolone	154000	22435SI	59	20160225*
Caelo	Prednisolone	161343	22467	60	20160601*
Caelo	Prednisolone	161343	22467SI	44	20160601*
Caelo	Prednisolone	15400002	22783	40	20160225
Caelo	Prednisolone	15400002	22783SI	40	20160225
Caelo	Prednisolone	20001355	25192	40	20200528*
Caelo	Prednisolone	20001355	25192SI	40	20200528*
Euro OTC	Prednisolone	1212021-02	21604	60	1411270

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Prednisolone	1212021-02	21604SI	48	1411270
Euro OTC	Prednisolone	1501047-01	21849	60	AR-15-FG-015509-01
Euro OTC	Prednisolone	1501047-01	21849SI	30	AR-15-FG-015509-01
Euro OTC	Prednisolone	1607011	22709	40	20160818*
Euro OTC	Prednisolone	1607011	22709SI	40	20160818*
Euro OTC	Prednisolone	2104012	25688	50	20210504*
Euro OTC	Prednisolone	2104012	25688SI	50	20210504*
Fagron	Prednisolone	13H07-B02-285592	21660	60	20130909
Fagron	Prednisolone	13H07-B02-285592	21660SI	60	20130909
Fagron	Prednisolone	14I10-B03-302263	22651	40	20141020
Fagron	Prednisolone	14I10-B03-302263	22651SI	40	20141020
Fagron	Prednisolone	16C15-B01-320761	22803	40	20160407
Fagron	Prednisolone	16C15-B01-320761	22803SI	36	20160407

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1176 spectra of 25 reference samples from the substance/substance group *Prednisolone*. These samples are listed above in the *calibration samples* section. The reference samples come from 14 different batches.
- 151 786 spectra from a total of 2828 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 852 spectra of 23 reference samples from the substance/substance group *Prednisolone*.
- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Prednisolone	172777	23846	40
Caelo	Prednisolone	21003654002	26414	40
Euro OTC	Prednisolone	1702020	23180	40
Euro OTC	Prednisolone	1905005	24602	40
Euro OTC	Prednisolone	2003019	25243	40
Euro OTC	Prednisolone	2205002	26208	40
Euro OTC	Prednisolone	2401004	27090	40
Fagron	Prednisolone	1108055-04	20855	40
Fagron	Prednisolone	16E09-B07-328220	23260	40
Fagron	Prednisolone	22B07-B20-220068	26289	30
Fagron	Prednisolone	24C07-B05-238310	27264	40
Caelo	Prednisolone	13343105	21451SI	60
Caelo	Prednisolone	161343	22467SI†	3
Caelo	Prednisolone	172777	23846SI	38
Caelo	Prednisolone	21003654002	26414SI	40
Euro OTC	Prednisolone	1702020	23180SI	21
Euro OTC	Prednisolone	1905005	24602SI	40
Euro OTC	Prednisolone	2003019	25243SI	40
Euro OTC	Prednisolone	2205002	26208SI	40
Euro OTC	Prednisolone	2401004	27090SI	40
Fagron	Prednisolone	16E09-B07-328220	23260SI	20
Fagron	Prednisolone	22B07-B20-220068	26289SI	40
Fagron	Prednisolone	24C07-B05-238310	27264SI	40

- 201 232 spectra from a total of 4032 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2806 spectra from 941 *Apo-Ident* customers from 479 batches from the substance/substance group *Prednisolone*.

- Among them are spectra of independent samples from 453 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Prednisolone	1702020-02	1
	Prednisolone	21003654007	2
	Prednisolone	21003654010	1
	Prednisolone	21003654014	1
	Prednisolone	21003654016	2
	Prednisolone	21003654017	2
	Prednisolone	21003654021	5
	Prednisolone	2104012-01	2
	Prednisolone	21K27B04216441	1
	Prednisolone	2205002-01	14
	Prednisolone	22B07-B20-220050	2
	Prednisolone	22B07-B20-220068	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Prednisolone	22B07-B21	1
	Prednisolone	22B07-B21-222188	3
	Prednisolone	22B07-B21-222189	2
	Prednisolone	22B07-B21-224306	1
	Prednisolone	23002419002	2
	Prednisolone	23002419003	5
	Prednisolone	23002419006	3
	Prednisolone	23D24-B06-227228	3
	Prednisolone	23D24-B06-233604	2
	Prednisolone	2401004-01	1
	Prednisolone	B04-2336002	3
A.H. 05.03.13 ek: 14,08EUR	Prednisolone	12D30-N04	1
Aep	Prednisolone	21003654017	1
AHD/EuRho	Prednisolone	1905005-01	1
AHD	Prednisolone	121202103	1
AHD	Prednisolone	1212021-03	1
AHD	Prednisolone	160711-01	1
AHD	Prednisolone	16134308	1
AHD	Prednisolone	16134316	1
AHD	Prednisolone	1702020-01	1
AHD	Prednisolone	17277706	1
AHD	Prednisolone	21K27-B04-216441	2
AHD	Prednisolone	22B07-B21-222189	1
AHD	Prednisolone	23002419003	1
AHD	Prednisolone	24C07-B05-238309	1
Alliance Healtcare	Prednisolone	21003654002	1
Alliance Healthcare	Prednisolone	172777004	1
Alliance Healthcare	Prednisolone	17277723	1
Alliance Healthcare	Prednisolone	20001355002	1
Alliance Healthcare	Prednisolone	20004564006	2
Alliance Healthcare	Prednisolone	21003654012	1
Alliance Healthcare	Prednisolone	2205002-01	2
anzag	Prednisolone	14B18-B05-294966	1
Anzag	Prednisolone	20004564003	1
apo-Ident/ Sanacorp	Prednisolone	K04120190707	1
apomix	Prednisolone	16H04-B03-332930	1
Apotheke Mildenau	Prednisolone	1108055-04	3
Beiersdorf	Prednisolone	20004564003	1
Berkel AHK	Prednisolone	13343115	1
Bomastus / Alliance ...	Prednisolone	16134305	1
Bombastus	Prednisolone	1501047-02	1
Bombastus	Prednisolone	17F07-B05-341574	2
Bombastus	Prednisolone	17F07-B05-341578	2
Caelo	Prednisolone		2
Caelo	Prednisolone	10196604	1
Caelo	Prednisolone	10196606	1
Caelo	Prednisolone	10196611	3
Caelo	Prednisolone	10196622	2
Caelo	Prednisolone	10196625	1
Caelo	Prednisolone	10196626	6
Caelo	Prednisolone	10196627	7
Caelo	Prednisolone	11/26-N04	1
Caelo	Prednisolone	1212021-01	1
Caelo	Prednisolone	121202102	1
Caelo	Prednisolone	1212021-03	6
Caelo	Prednisolone	12171301	6
Caelo	Prednisolone	12171302	1
Caelo	Prednisolone	12171303	2
Caelo	Prednisolone	12171306	2
Caelo	Prednisolone	12185702	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednisolone	1232417	1
Caelo	Prednisolone	12324202	11
Caelo	Prednisolone	12324203	3
Caelo	Prednisolone	12324204	4
Caelo	Prednisolone	12324205	13
Caelo	Prednisolone	12324207	4
Caelo	Prednisolone	12324213	7
Caelo	Prednisolone	12324216	9
Caelo	Prednisolone	12324217	5
Caelo	Prednisolone	12324219	7
Caelo	Prednisolone	12324220	2
Caelo	Prednisolone	12324221	2
Caelo	Prednisolone	12324226	7
Caelo	Prednisolone	1234205	1
Caelo	Prednisolone	1234556	1
Caelo	Prednisolone	1250216	1
Caelo	Prednisolone	133414	1
Caelo	Prednisolone	13343101	1
Caelo	Prednisolone	13343104	11
Caelo	Prednisolone	13343105	4
Caelo	Prednisolone	13343106	8
Caelo	Prednisolone	13343107	1
Caelo	Prednisolone	13343111	4
Caelo	Prednisolone	13343112	4
Caelo	Prednisolone	13343113	1
Caelo	Prednisolone	13343114	5
Caelo	Prednisolone	13343115	9
Caelo	Prednisolone	13343116	4
Caelo	Prednisolone	13A07-N14	1
Caelo	Prednisolone	13E15-N06	4
Caelo	Prednisolone	14/10B03302265	1
Caelo	Prednisolone	14/10-B03-302266	1
Caelo	Prednisolone	1410B03302265	1
Caelo	Prednisolone	14A30-B02-294968	1
Caelo	Prednisolone	14B18-B05-294966	2
Caelo	Prednisolone	14G30-B14-302262	2
Caelo	Prednisolone	150104701	2
Caelo	Prednisolone	1501047-01	3
Caelo	Prednisolone	1501047-02	3
Caelo	Prednisolone	15055101	7
Caelo	Prednisolone	15055102	6
Caelo	Prednisolone	15055105	1
Caelo	Prednisolone	1511011	1
Caelo	Prednisolone	152006105	1
Caelo	Prednisolone	15206101	9
Caelo	Prednisolone	15206102	19
Caelo	Prednisolone	15206103	12
Caelo	Prednisolone	15206105	8
Caelo	Prednisolone	15206106	1
Caelo	Prednisolone	15206108	14
Caelo	Prednisolone	15400001	5
Caelo	Prednisolone	15400002	21
Caelo	Prednisolone	15400003	28
Caelo	Prednisolone	15400004	26
Caelo	Prednisolone	15400010	8
Caelo	Prednisolone	1540003	1
Caelo	Prednisolone	15K03-B04-314358	1
Caelo	Prednisolone	16034301	2
Caelo	Prednisolone	1607011-01	4
Caelo	Prednisolone	1613414	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednisolone	161343001	1
Caelo	Prednisolone	16134301	11
Caelo	Prednisolone	16134302	20
Caelo	Prednisolone	16134303	2
Caelo	Prednisolone	161343032	1
Caelo	Prednisolone	16134305	23
Caelo	Prednisolone	16134306	4
Caelo	Prednisolone	16134308	14
Caelo	Prednisolone	16134310	34
Caelo	Prednisolone	16134310-28122017/1	1
Caelo	Prednisolone	16134314	25
Caelo	Prednisolone	16134314/2120418	1
Caelo	Prednisolone	16134315	26
Caelo	Prednisolone	16134316	23
Caelo	Prednisolone	161343215	1
Caelo	Prednisolone	16A20-B03-316421	1
Caelo	Prednisolone	16C15-B01_320761	1
Caelo	Prednisolone	16C15-B01-320761	1
Caelo	Prednisolone	16C15-B01-321979	2
Caelo	Prednisolone	16C15-B01-324942	1
Caelo	Prednisolone	16C15-B02-324943	1
Caelo	Prednisolone	16E09-B07-328150	3
Caelo	Prednisolone	16E09-B07-328220	1
Caelo	Prednisolone	17020-01	1
Caelo	Prednisolone	1702020-01	3
Caelo	Prednisolone	1702020-02	3
Caelo	Prednisolone	1702020-03	3
Caelo	Prednisolone	172277710	1
Caelo	Prednisolone	17277004	1
Caelo	Prednisolone	1727702	2
Caelo	Prednisolone	1727704	2
Caelo	Prednisolone	1727710	1
Caelo	Prednisolone	1727716	2
Caelo	Prednisolone	1727718	1
Caelo	Prednisolone	1727720	1
Caelo	Prednisolone	1727723	1
Caelo	Prednisolone	1727770	1
Caelo	Prednisolone	172777002	35
Caelo	Prednisolone	17277702	13
Caelo	Prednisolone	17277703	15
Caelo	Prednisolone	17277704	42
Caelo	Prednisolone	17277706	18
Caelo	Prednisolone	17277710	14
Caelo	Prednisolone	17277711	24
Caelo	Prednisolone	17277714	1
Caelo	Prednisolone	17277716	42
Caelo	Prednisolone	17277718	3
Caelo	Prednisolone	17277719	1
Caelo	Prednisolone	17277720	33
Caelo	Prednisolone	17277723	16
Caelo	Prednisolone	1727777723	1
Caelo	Prednisolone	177277703	1
Caelo	Prednisolone	17f07-b05	1
Caelo	Prednisolone	17F07B05341574	1
Caelo	Prednisolone	17F07-B05-341574	2
Caelo	Prednisolone	17F07-B05-341578	1
Caelo	Prednisolone	18138113	1
Caelo	Prednisolone	18A29-B02-348041	1
Caelo	Prednisolone	18A29-B02-348540	2
Caelo	Prednisolone	18H07-B04-354523	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednisolone	18H07-B04-355631	2
Caelo	Prednisolone	1905005-01	2
Caelo	Prednisolone	1905005-02	1
Caelo	Prednisolone	19081504	1
Caelo	Prednisolone	20001355001	4
Caelo	Prednisolone	20001355002	13
Caelo	Prednisolone	20001355003	16
Caelo	Prednisolone	200013555002	1
Caelo	Prednisolone	20004564001	1
Caelo	Prednisolone	20004564002	6
Caelo	Prednisolone	20004564003	30
Caelo	Prednisolone	20004564005	24
Caelo	Prednisolone	20004564006	9
Caelo	Prednisolone	20004564008	7
Caelo	Prednisolone	20004564009	17
Caelo	Prednisolone	20021303	1
Caelo	Prednisolone	2004564002	1
Caelo	Prednisolone	20H20-B01-200829	1
Caelo	Prednisolone	21003645002	1
Caelo	Prednisolone	21003654002	21
Caelo	Prednisolone	21003654004	12
Caelo	Prednisolone	21003654006	1
Caelo	Prednisolone	21003654007	3
Caelo	Prednisolone	21003654010	7
Caelo	Prednisolone	21003654012	4
Caelo	Prednisolone	21003654014	2
Caelo	Prednisolone	21003654016	1
Caelo	Prednisolone	21003654017	2
Caelo	Prednisolone	21E04-B02-215330	1
Caelo	Prednisolone	21EO4-BO2-215330	1
Caelo	Prednisolone	21K27-B04-216439	3
Caelo	Prednisolone	22BO7-B20-220068	1
Caelo	Prednisolone	2413Q02105	1
Caelo	Prednisolone	3344	1
Caelo	Prednisolone	411092-1-P	1
Caelo	Prednisolone	4513U2105	1
Caelo	Prednisolone	4712I-02105	1
Caelo	Prednisolone	60367086	2
Caelo	Prednisolone	702020-01	1
Caelo	Prednisolone	9193501	1
Caelo	Prednisolone	AP201025-04	1
Caelo	Prednisolone	I-180716-15400003	1
Caelo	Prednisolone	I220216/2	1
Caelo	Prednisolone	k04c20121219	1
Caelo	Prednisolone	NEPL160202	1
Caelo	Prednisolone	NEPL180603	1
Caesar & Lorenz GmbH	Prednisolone	172777002	1
Caesar & Lorenz	Prednisolone	21003654012	1
Caesar & Loretz GmbH…	Prednisolone	172777002	1
Caesar & Loretz GmbH…	Prednisolone	17277720	1
Caesar & Loretz GmbH…	Prednisolone	20001355003	1
Caesar & Loretz GmbH…	Prednisolone	17277720	1
Caesar & Loretz GmbH…	Prednisolone	17277720	1
Caesar & Loretz GmbH…	Prednisolone	21003654010	1
Caesar & Loretz GmbH…	Prednisolone	17277718	2
Caesar & Loretz GmbH, Now	Prednisolone	21003654012	1
Caesar & Loretz GmbH…	Prednisolone	17277720	1
Caesar & Loretz GmbH/GEHE	Prednisolone	172777002	1
Caesar & Loretz GmbH/Gehe	Prednisolone	17277710	3
Caesar & Loretz GmbH/Gehe	Prednisolone	21003654017	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Prednisolone	17277711	1
Caesar & Loretz GmbH...	Prednisolone	20004564005	1
Caesar & Loretz GmbH/Kehr	Prednisolone	17277710	1
Caesar & Loretz GmbH...	Prednisolone	17277711	1
Caesar & Loretz GmbH...	Prednisolone	20001355002	1
Caesar & Loretz GmbH...	Prednisolone	21003654002	1
Caesar & Loretz GmbH...	Prednisolone	20004564005	1
Caesar & Loretz GmbH...	Prednisolone	17277720	1
Caesar & Loretz GmbH...	Prednisolone	20001355003	1
Caesar & Loretz GmbH...	Prednisolone	20004564009	1
Caesar & Loretz GmbH...	Prednisolone	B09-1977207	1
Caesar & Loretz GmbH...	Prednisolone	17277723	1
Caesar & Loretz GmbH...	Prednisolone	1905005-01	1
Caesar & Loretz GmbH...	Prednisolone	20001355002	1
Caesar & Loretz GmbH...	Prednisolone	20004564003	1
Caesar & Loretz GmbH...	Prednisolone	20001355002	1
Caesar & Loretz GmbH	Prednisolone	12324205	1
Caesar & Loretz GmbH	Prednisolone	12324219	1
Caesar & Loretz GmbH	Prednisolone	15206101	2
Caesar & Loretz GmbH	Prednisolone	172777002	14
Caesar & Loretz GmbH	Prednisolone	172777004	1
Caesar & Loretz GmbH	Prednisolone	17277702	2
Caesar & Loretz GmbH	Prednisolone	17277704	4
Caesar & Loretz GmbH	Prednisolone	17277706	2
Caesar & Loretz GmbH	Prednisolone	17277710	1
Caesar & Loretz GmbH	Prednisolone	17277711	8
Caesar & Loretz GmbH	Prednisolone	17277716	11
Caesar & Loretz GmbH	Prednisolone	17277718	2
Caesar & Loretz GmbH	Prednisolone	17277720	12
Caesar & Loretz GmbH	Prednisolone	17277723	9
Caesar & Loretz GmbH	Prednisolone	190500502	1
Caesar & Loretz GmbH	Prednisolone	20001355002	5
Caesar & Loretz GmbH	Prednisolone	20001355003	6
Caesar & Loretz GmbH	Prednisolone	20004564002	7
Caesar & Loretz GmbH	Prednisolone	20004564003	10
Caesar & Loretz GmbH	Prednisolone	20004564005	11
Caesar & Loretz GmbH	Prednisolone	20004564006	7
Caesar & Loretz GmbH	Prednisolone	20004564008	5
Caesar & Loretz GmbH	Prednisolone	20004564009	10
Caesar & Loretz GmbH	Prednisolone	21003654002	7
Caesar & Loretz GmbH	Prednisolone	21003654004	6
Caesar & Loretz GmbH	Prednisolone	21003654007	2
Caesar & Loretz GmbH	Prednisolone	21003654010	4
Caesar & Loretz GmbH	Prednisolone	21003654012	1
Caesar & Loretz GmbH	Prednisolone	21003654014	2
Caesar & Loretz GmbH	Prednisolone	21003654021	1
Caesar & Loretz Hild...	Prednisolone	17277723	1
Caesar & Loretz Hilden	Prednisolone	17277711	1
Caesar & Loretz Hilden	Prednisolone	17277716	1
Caesar & Loretz Hilden	Prednisolone	20001355003	1
Caesar & Loretz	Prednisolone	20001355002	2
Caesar u. Loretz/Noweda	Prednisolone	16134301	1
Caesar&Loretz GmbH/Anzag	Prednisolone	13343112	1
Caesar/Lorenz	Prednisolone	12324204	1
Caesar+ Loretz GmbH	Prednisolone	20004564003	1
Caleo/Jenne 28.04.22...	Prednisolone	20004564006	1
Caolo- Noweda	Prednisolone	15206103	1
Cealo/Noweda	Prednisolone	1526108	1
Cealo	Prednisolone	16134305	2
Cealo	Prednisolone	17277703	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Cealo	Prednisolone	2001355002	1
Cealo	Prednisolone	21003654002	1
Celo/Noweda	Prednisolone	1727703	1
CVH/Jenne	Prednisolone	19K27-B09	1
Ebert & Jacobi	Prednisolone	1212021-03	2
EU.RHO.Pharm	Prednisolone	K04120190707	1
EuRho/AHD	Prednisolone	1702020-03	1
EuRho/Jenne	Prednisolone	1108055-04	2
EuRho/Noweda	Prednisolone	1702020-01	1
EuRho	Prednisolone	1012012-01	1
EuRho	Prednisolone	1012012-02	2
EuRho	Prednisolone	1108055-03	2
EuRho	Prednisolone	1212021-02	1
EuRho	Prednisolone	1702020-01	1
EuRho	Prednisolone	1702020-02	1
EuRho	Prednisolone	190500501	1
EuRho	Prednisolone	2003019-01	1
Euro Gehe	Prednisolone	1702020-03	1
Euro OCT/Noweda	Prednisolone	1501047-02	1
Euro OTC	Prednisolone		1
Euro OTC	Prednisolone	1012012-02	2
Euro OTC	Prednisolone	1108055-01	1
Euro OTC	Prednisolone	1108055-02	2
Euro OTC	Prednisolone	1108055-03	10
Euro OTC	Prednisolone	110805504	4
Euro OTC	Prednisolone	1108055-04	17
Euro OTC	Prednisolone	118055-04	1
Euro OTC	Prednisolone	12021-03	1
Euro OTC	Prednisolone	121021-01	2
Euro OTC	Prednisolone	1212021	1
Euro OTC	Prednisolone	121202101	1
Euro OTC	Prednisolone	1212021-01	30
Euro OTC	Prednisolone	121202102	2
Euro OTC	Prednisolone	1212021-02	27
Euro OTC	Prednisolone	1212021-03	40
Euro OTC	Prednisolone	121221-03	1
Euro OTC	Prednisolone	1314Q2105	1
Euro OTC	Prednisolone	13343104	1
Euro OTC	Prednisolone	14/10-B03-302263	1
Euro OTC	Prednisolone	1501047	1
Euro OTC	Prednisolone	150104701	3
Euro OTC	Prednisolone	1501047-01	27
Euro OTC	Prednisolone	1501047-02	18
Euro OTC	Prednisolone	1501047-03	6
Euro OTC	Prednisolone	150104743	1
Euro OTC	Prednisolone	150104747-01	1
Euro OTC	Prednisolone	15010477-01	1
Euro OTC	Prednisolone	1501074-02	1
Euro OTC	Prednisolone	15014047-02	1
Euro OTC	Prednisolone	15206108	1
Euro OTC	Prednisolone	15400010	1
Euro OTC	Prednisolone	15K03-B04-314226	1
Euro OTC	Prednisolone	1607011-01	42
Euro OTC	Prednisolone	16134308	3
Euro OTC	Prednisolone	16134316	2
Euro OTC	Prednisolone	16E09-B07-329686	2
Euro OTC	Prednisolone	170202001	2
Euro OTC	Prednisolone	1702020-01	55
Euro OTC	Prednisolone	170202002	3
Euro OTC	Prednisolone	1702020-02	52

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Prednisolone	1702020-03	25
Euro OTC	Prednisolone	170202-03	3
Euro OTC	Prednisolone	1702020-30	1
Euro OTC	Prednisolone	170202201	1
Euro OTC	Prednisolone	172020-03	1
Euro OTC	Prednisolone	18A29-B02-348044	1
Euro OTC	Prednisolone	18H07-B04	1
Euro OTC	Prednisolone	190500-01	2
Euro OTC	Prednisolone	19050005-01	1
Euro OTC	Prednisolone	1905005	1
Euro OTC	Prednisolone	1905005_01	1
Euro OTC	Prednisolone	190500501	6
Euro OTC	Prednisolone	1905005-01	85
Euro OTC	Prednisolone	1905005-02	30
Euro OTC	Prednisolone	1905005-0P-191223-5	1
Euro OTC	Prednisolone	190500t-02	1
Euro OTC	Prednisolone	200301901	2
Euro OTC	Prednisolone	2003019-01	44
Euro OTC	Prednisolone	200560	1
Euro OTC	Prednisolone	210401201	1
Euro OTC	Prednisolone	2104012-01	20
Euro OTC	Prednisolone	30042014B	1
Euro OTC	Prednisolone	501047-01	1
Euro OTC	Prednisolone	NEPL110103	1
Euro/ Sanacorp	Prednisolone	121202103	1
Euro/Gehe	Prednisolone	1702020-01	1
Euro/Phoenix	Prednisolone	190500501	1
Euro/Phoenix	Prednisolone	190500502	1
Euro/Phönix	Prednisolone	1702020-01	1
Euro/Phönix	Prednisolone	1905005-01	1
euroct/gehe	Prednisolone	1212021-01	1
euroct/Gehe	Prednisolone	1212021-01	1
Europh/Ph	Prednisolone	1702020-02	1
Europharm/Otto	Prednisolone	1108055-03	1
Europharm/Otto	Prednisolone	1108055-04	5
europharma	Prednisolone	1002001240	1
Fagron	Prednisolone		1
Fagron	Prednisolone	10J04-N06	1
Fagron	Prednisolone	11D13-N05	2
Fagron	Prednisolone	11G22-N08	1
Fagron	Prednisolone	11J26-N04	2
Fagron	Prednisolone	1212021-02	2
Fagron	Prednisolone	12324216	1
Fagron	Prednisolone	12c22-N05	1
Fagron	Prednisolone	12C22-N05	7
Fagron	Prednisolone	12D30-N04	9
Fagron	Prednisolone	12D30-NO4	1
Fagron	Prednisolone	12K14-N03	10
Fagron	Prednisolone	12K14-NO3	1
Fagron	Prednisolone	130F-N04	1
Fagron	Prednisolone	13343106	1
Fagron	Prednisolone	13A07N14	1
Fagron	Prednisolone	13A07-N14	6
Fagron	Prednisolone	13DE15-N06	1
Fagron	Prednisolone	13E13-N06	1
Fagron	Prednisolone	13E15-N06	16
Fagron	Prednisolone	13E15-NO6	1
Fagron	Prednisolone	13G03-B09	1
Fagron	Prednisolone	13H07-B02	2
Fagron	Prednisolone	13H07-B020	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednisolone	13H07-B02-285590	3
Fagron	Prednisolone	13H07-B02-285592	4
Fagron	Prednisolone	13H07-B02-285593	4
Fagron	Prednisolone	13H07-B02-285593	1
Fagron	Prednisolone	13H7-B02-285590	1
Fagron	Prednisolone	13J28-B06	2
Fagron	Prednisolone	13J28-B06-289670	3
Fagron	Prednisolone	14/10-B03	1
Fagron	Prednisolone	14/10B03302265	1
Fagron	Prednisolone	14/10-B03-302265	4
Fagron	Prednisolone	14/10-B03-302266	2
Fagron	Prednisolone	14/10-B03-302269	1
Fagron	Prednisolone	14/10-B03-302271	1
Fagron	Prednisolone	1410-B03	1
Fagron	Prednisolone	1410-B03-302269	2
Fagron	Prednisolone	14818-B05-294966	1
Fagron	Prednisolone	14A30-B02-294968	5
Fagron	Prednisolone	14B18-B05	1
Fagron	Prednisolone	14B18-B05294966	1
Fagron	Prednisolone	14B18-B05-294966	10
Fagron	Prednisolone	14B18-B05-294969	2
Fagron	Prednisolone	14B18-Bo5-294966	1
Fagron	Prednisolone	14G30-B14	1
Fagron	Prednisolone	14G30-B14-302262	4
Fagron	Prednisolone	14I10-B03	1
Fagron	Prednisolone	14I10-B03-302265	2
Fagron	Prednisolone	14I10-B03-302266	1
Fagron	Prednisolone	14i10-b03-302269	1
Fagron	Prednisolone	14I10-B03-302269	3
Fagron	Prednisolone	14l10-B03302265	1
Fagron	Prednisolone	14L10-B03-302269	1
Fagron	Prednisolone	1501047-02	1
Fagron	Prednisolone	150528P	1
Fagron	Prednisolone	15B18-B05-294969	1
Fagron	Prednisolone	15D14-B01	1
Fagron	Prednisolone	15D14-B01-308425	3
Fagron	Prednisolone	15K03_B04_314226	1
Fagron	Prednisolone	15K03-B04	1
Fagron	Prednisolone	15k03-b04-314226	1
Fagron	Prednisolone	15K03B04314226	1
Fagron	Prednisolone	15K03-B04-314226	13
Fagron	Prednisolone	15K03-B04-314357	2
Fagron	Prednisolone	15K03-B04-314358	6
Fagron	Prednisolone	15K03-B04-314869	2
Fagron	Prednisolone	15KO3-B04-314226	1
Fagron	Prednisolone	1607011-01	2
Fagron	Prednisolone	16134310	1
Fagron	Prednisolone	16A20-B03	4
Fagron	Prednisolone	16A20-B03-316420	7
Fagron	Prednisolone	16A20-B03-316421	1
Fagron	Prednisolone	16A20-B03-319015	7
Fagron	Prednisolone	16c15-802	1
Fagron	Prednisolone	16C15-B01	1
Fagron	Prednisolone	16C15-B01-319992	2
Fagron	Prednisolone	16c15-B01-320761	2
Fagron	Prednisolone	16C15B01320761	2
Fagron	Prednisolone	16C15-B01-320761	4
Fagron	Prednisolone	16C15B01321979	1
Fagron	Prednisolone	16C15-B01-321979	15
Fagron	Prednisolone	16C15-B01-324942	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednisolone	16c15-b02	1
Fagron	Prednisolone	16C15-B02	1
Fagron	Prednisolone	16C15-B02-324943	6
Fagron	Prednisolone	16C15-B02-324945	1
Fagron	Prednisolone	16C15-B01-321979	1
Fagron	Prednisolone	16C19-B07-353242	1
Fagron	Prednisolone	16E09/B07/328220	1
Fagron	Prednisolone	16E09-B07_328220	1
Fagron	Prednisolone	16E09-B07-328150	17
Fagron	Prednisolone	16E09-B07-328220	7
Fagron	Prednisolone	16e09-B07-329686	1
Fagron	Prednisolone	16E09-B07-329686	1
Fagron	Prednisolone	16E09-B075411	1
Fagron	Prednisolone	16H04b03332929	1
Fagron	Prednisolone	16H04-B03-332929	15
Fagron	Prednisolone	16H04-B03-332930	8
Fagron	Prednisolone	16K27-B09-200489	1
Fagron	Prednisolone	17014-801-340448	1
Fagron	Prednisolone	17020201	1
Fagron	Prednisolone	1711021A	1
Fagron	Prednisolone	1717M-02105	1
Fagron	Prednisolone	17D14-B01	1
Fagron	Prednisolone	17D14b01338573	1
Fagron	Prednisolone	17D14-B01-338573	5
Fagron	Prednisolone	17D14-Bo1-338573	1
Fagron	Prednisolone	17F07-B05	3
Fagron	Prednisolone	17F07-B05_341574	1
Fagron	Prednisolone	17F07-B05-341574	6
Fagron	Prednisolone	17F07-B05-341575	5
Fagron	Prednisolone	17F07-B05-341578	2
Fagron	Prednisolone	17g2828-b03-345539	1
Fagron	Prednisolone	17G28-B03	3
Fagron	Prednisolone	17G28-B03-345538	10
Fagron	Prednisolone	17G28-B03-345539	4
Fagron	Prednisolone	17G2B03-345538	1
Fagron	Prednisolone	18A29-B02	2
Fagron	Prednisolone	18A29-B02-348041	2
Fagron	Prednisolone	18A29-B02-348044	1
Fagron	Prednisolone	18A29-B02-348540	4
Fagron	Prednisolone	18C19-B07	2
Fagron	Prednisolone	18C19-B07-351225	5
Fagron	Prednisolone	18C19B07351226	1
Fagron	Prednisolone	18C19-B07-351226	4
Fagron	Prednisolone	18C19-B07-353242	5
Fagron	Prednisolone	18H07-804	1
Fagron	Prednisolone	18H07-B04	3
Fagron	Prednisolone	18H07-B04_355630	1
Fagron	Prednisolone	18h07-b04-353326	1
Fagron	Prednisolone	18H07-B04-353326	4
Fagron	Prednisolone	18H07-B04-354523	10
Fagron	Prednisolone	18H07-B04-355630	6
Fagron	Prednisolone	18H07B04355631	1
Fagron	Prednisolone	18H07-B04-355631	6
Fagron	Prednisolone	18H7-B04-355631	1
Fagron	Prednisolone	1905005-01	3
Fagron	Prednisolone	194548	1
Fagron	Prednisolone	19-B07-351226	1
Fagron	Prednisolone	19E28-814-191220	1
Fagron	Prednisolone	19e28-B13	1
Fagron	Prednisolone	19E28-B13	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednisolone	19E28B13191224	1
Fagron	Prednisolone	19E28-B13-191224	9
Fagron	Prednisolone	19E28-B14	3
Fagron	Prednisolone	19E28-B14-1911225	1
Fagron	Prednisolone	19E28-B14-191220	16
Fagron	Prednisolone	19E28-B14-1912220	1
Fagron	Prednisolone	19H19-302	1
Fagron	Prednisolone	19H19-B02	3
Fagron	Prednisolone	19H19-B02-194547	1
Fagron	Prednisolone	19H19-B02-194548	10
Fagron	Prednisolone	19H19-B02-194549	2
Fagron	Prednisolone	19H19-BO2-194548	2
Fagron	Prednisolone	19K27-809	1
Fagron	Prednisolone	19K27-B09	2
Fagron	Prednisolone	19K27-B09-1977207	1
Fagron	Prednisolone	19k27b09197727	1
Fagron	Prednisolone	19K27-B09-197727	14
Fagron	Prednisolone	19k27-b09-200489	1
Fagron	Prednisolone	19K27B09-200489	1
Fagron	Prednisolone	19K27-B09-200489	10
Fagron	Prednisolone	19K27B09200517	2
Fagron	Prednisolone	19K27-B09-200517	6
Fagron	Prednisolone	20004564003	1
Fagron	Prednisolone	200738	1
Fagron	Prednisolone	20H20-B01	2
Fagron	Prednisolone	20H20-B01_202715	1
Fagron	Prednisolone	20H20B01200714	1
Fagron	Prednisolone	20H20-B01-200736	1
Fagron	Prednisolone	20H20-B01-200738	7
Fagron	Prednisolone	20h20B01-200829	1
Fagron	Prednisolone	20H20-B01-200829	3
Fagron	Prednisolone	20H20-B01-202715	6
Fagron	Prednisolone	20H20-B01-204241	2
Fagron	Prednisolone	20H20-BO1-200829	1
Fagron	Prednisolone	21/07-B03-213752	1
Fagron	Prednisolone	21107-B03	1
Fagron	Prednisolone	211217(19519-B02-194548)	1
Fagron	Prednisolone	21E04-B02215330	2
Fagron	Prednisolone	21E04-B02-215330	10
Fagron	Prednisolone	21I07B03213148	1
Fagron	Prednisolone	21I07-B03-213148	1
Fagron	Prednisolone	21I07-B03-213752	5
Fagron	Prednisolone	21k27-b04-216439	1
Fagron	Prednisolone	21K27-B04-216439	5
Fagron	Prednisolone	21K27-BO4-216441	1
Fagron	Prednisolone	22807-820-220050	1
Fagron	Prednisolone	22B07-B20-220050	2
Fagron	Prednisolone	22b07-B21-222188	1
Fagron	Prednisolone	23E30-B04-234317	1
Fagron	Prednisolone	2834	1
Fagron	Prednisolone	2915E-02105	1
Fagron	Prednisolone	3518E-02105	1
Fagron	Prednisolone	4313E-02105	1
Fagron	Prednisolone	613Q-02105	1
Fagron	Prednisolone	8576886	1
Fagron	Prednisolone	B01-2007308	1
Fagron	Prednisolone	B01-2008209	2
Fagron	Prednisolone	B02-1945408	1
Fagron	Prednisolone	B02-2153300	1
Fagron	Prednisolone	B09-1977207	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednisolone	B09-1977208	1
Fagron	Prednisolone	B09-2004809	2
Fagron	Prednisolone	b14-1912200	1
Fagron	Prednisolone	BO9-1977207	1
Fagron	Prednisolone	K04C20121006	1
Fagron	Prednisolone	K04C20130203M	1
Fagron	Prednisolone	K04C20131102	1
Fagron	Prednisolone	K04C20140502	2
Fagron	Prednisolone	KO4C20121006	1
Fagron	Prednisolone	NEPL151202	1
Fagron	Prednisolone	NEPL160202	1
Fagron	Prednisolone	NEPL160705	1
Fagron	Prednisolone	NEPL170209	2
Fagron	Prednisolone	NEPL170210	1
Fagron	Prednisolone	NEPL170605	3
Fagron	Prednisolone	NEPL1711	1
Fagron	Prednisolone	NEPL171111	1
Fagron	Prednisolone	NEPL180603	1
Fagron	Prednisolone	NEPL190306	1
Fagron	Prednisolone	NEPL190405	4
Fagron	Prednisolone	nepl190811	1
Fagron	Prednisolone	NEPL190811	2
Fagron	Prednisolone	NEPL200714	1
Fagron	Prednisolone	NEPL211006	2
Fagron	Prednisolone	NPL190306	1
Fargo	Prednisolone	12D30-N04	1
Fargon / AHD	Prednisolone	18C19-B07-351226	1
Fargon/AHD	Prednisolone	18A29-B02-348044	1
Fargon/Kehr	Prednisolone	22B07-B21-224304	1
Fargon	Prednisolone	16134308	1
Fargon	Prednisolone	19E28-B14-191220	1
Fargon	Prednisolone	FPO1409P	1
Fargron	Prednisolone	13E15-N06	1
Fischar/Gehe	Prednisolone	14A30-B02-294968	1
Fragon/Phoenix	Prednisolone	15K03-B04-314226	1
Fragon/Phoenix	Prednisolone	16C15-B02-324943	1
Fragon	Prednisolone	18C19-B07-351225	1
Gehe amax	Prednisolone	1501047-01	3
Gehe amax	Prednisolone	1607011-01	2
Gehe amax	Prednisolone	16134310	1
Gehe amax	Prednisolone	1702020-01	1
Gehe amax	Prednisolone	1702020-02	1
Gehe amax	Prednisolone	17277704	1
Gehe amax	Prednisolone	17277720	2
Gehe amax	Prednisolone	1905005-01	2
Gehe/Fragon	Prednisolone	16E09B07328150	1
Gehe	Prednisolone	1212021-01	4
Gehe	Prednisolone	1212021-02	1
Gehe	Prednisolone	12324216	2
Gehe	Prednisolone	12C22-N05	1
Gehe	Prednisolone	13343107	1
Gehe	Prednisolone	13A07-N14	2
Gehe	Prednisolone	13E15-No6	1
Gehe	Prednisolone	14A30-B02-294968	1
Gehe	Prednisolone	1501047-01	4
Gehe	Prednisolone	16134302	1
Gehe	Prednisolone	16134314	1
Gehe	Prednisolone	16C15-B01	1
Gehe	Prednisolone	16C15-B01-321979	1
Gehe	Prednisolone	16C-15-B02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Prednisolone	16E09-B07	1
GEHE	Prednisolone	1702020-02	1
Gehe	Prednisolone	172777002	1
Gehe	Prednisolone	17277710	1
Gehe	Prednisolone	17277718	3
Gehe	Prednisolone	17F07-B05-341574	1
Gehe	Prednisolone	17G28-B03	1
Gehe	Prednisolone	18H07-B04	1
Gehe	Prednisolone	18H07-B04-355630	2
Gehe	Prednisolone	18H07-B04-355631	1
Gehe	Prednisolone	19E28-B14_191220	1
Gehe	Prednisolone	19H19-B02	1
Gehe	Prednisolone	20004564002	1
GEHE	Prednisolone	21K27-B04-216441	1
Gehe	Prednisolone	23E30-B04-235950	1
Gehe-Fragon	Prednisolone	14B18B05294966	1
GUMO	Prednisolone	19K27-B09_20048	1
Hedinger	Prednisolone	P2018/116	1
Henan / Ebert	Prednisolone	16134316	1
Henan Lihua/Gehe	Prednisolone	1501047-01	2
Henan/Noweda	Prednisolone	K04120190303	1
Ichthyol / Phoenix	Prednisolone	16C15-B01-320761	1
Ichthyol gesellschaft	Prednisolone	15400003	1
Jenne / Fargon	Prednisolone	14B18B05294966	2
Kehr	Prednisolone	23D24-B06-227228	1
Kehr	Prednisolone	23D24-B06-227230	1
Krieger	Prednisolone	3416	1
Leyh Pharma	Prednisolone	16A20-B03-319015	1
Nachprüfung	Prednisolone	2082019-8	1
Noweda	Prednisolone	10196626	2
Noweda	Prednisolone	1108055-05	1
Noweda	Prednisolone	1212021-02	1
Noweda	Prednisolone	15206101	1
Noweda	Prednisolone	1607011-01	1
Noweda	Prednisolone	16134316	1
Noweda	Prednisolone	16H04-B03-332930	1
Noweda	Prednisolone	18A29-B02-348041	1
Noweda	Prednisolone	1905005-01	1
Noweda	Prednisolone	19E28-B14-191220	2
Noweda	Prednisolone	20004564003	1
Noweda	Prednisolone	20004564005	1
Noweda	Prednisolone	20H20-B01-200829	1
Noweda	Prednisolone	21003654002	1
Noweda	Prednisolone	21107-B03-213752	1
Noweda	Prednisolone	2205002-01	5
Noweda-Euro	Prednisolone	K04I20210211	2
Otto Geilenkirchen	Prednisolone	16134305	1
Ph.Eur 8.0	Prednisolone	14/10-B03-302263	2
Phoenix 01.08.2017 8,69EUR	Prednisolone	16E09-B07-328150	1
Phoenix 14.11.2017	Prednisolone	16H04-B03-332929	1
phoenix 5.4.2013	Prednisolone	1108055-04	1
Phoenix	Prednisolone	11j26-N04	2
Phoenix	Prednisolone	15400003	1
Phoenix	Prednisolone	16134310	1
Phoenix	Prednisolone	16134315	1
Phoenix	Prednisolone	16H04B03332930	1
Phoenix	Prednisolone	17277703	1
Phoenix	Prednisolone	17277711	1
Phoenix	Prednisolone	20004564005	4
Phoenix	Prednisolone	20004564009	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Prednisolone	200602406	1
Phoenix	Prednisolone	3220	1
Phönix Gotha	Prednisolone	1232417	1
Phönix Gotha	Prednisolone	12324213	1
Phönix Gotha	Prednisolone	12324217	1
Phönix Gotha	Prednisolone	13343105	1
Phönix Gotha	Prednisolone	13343111	1
Phönix Gotha	Prednisolone	13343112	2
Phönix/Euro	Prednisolone	1501047-03	1
Phönix/Euro	Prednisolone	1702020-02	1
Phönix/Fagon	Prednisolone	16C15-B01-324942	1
Phönix	Prednisolone	12324216	1
Phönix	Prednisolone	13A07N14	1
Phönix	Prednisolone	13E15-N06	2
Phönix	Prednisolone	14B18-B05-294966	1
Phönix	Prednisolone	16134305	1
Phönix	Prednisolone	16134314	1
Phönix	Prednisolone	17277704	1
phönix	Prednisolone	17277716	1
Phönix	Prednisolone	17277720	1
Phönix	Prednisolone	17277723	2
Phönix	Prednisolone	18A29B02348540	1
Phönix	Prednisolone	19K27-B09-200489	2
Phönix	Prednisolone	2003019-01	1
Röntgen	Prednisolone	170202001	1
Sanacorp WE:01.08.20…	Prednisolone	1501047-01	1
Sanacorp	Prednisolone	1108055-03	1
Sanacorp	Prednisolone	12324221	1
Sanacorp	Prednisolone	13343112	1
Sanacorp	Prednisolone	13E15-N06	1
Sanacorp	Prednisolone	13H07-B02-285592	1
Sanacorp	Prednisolone	13j28-b06-289670	1
sanacorp	Prednisolone	14/10-B03-302266	1
Sanacorp	Prednisolone	14/10-B03-302269	1
Sanacorp	Prednisolone	16134310	1
Sanacorp	Prednisolone	16H04-B03_332930	1
Sanacorp	Prednisolone	17F07-B05-341575	1
Sanacorp	Prednisolone	18AB02	1
Sanacorp	Prednisolone	20001355002	1
Sanacorp	Prednisolone	21I07-B03-213752	1
Sanacorp	Prednisolone	21K27-B04-0002	1
Sanacorp	Prednisolone	22B07-B20-220068	1
Sanacorp	Prednisolone	22B07-B21-224306	1
Sanacorp	Prednisolone	23002419002	1
Sanacorp	Prednisolone	23002419003	1
Sanacorp	Prednisolone	23E30-B04-235951	1
Sonnenberg-Apotheke	Prednisolone	12324219	1
Tianjin Tianyao Pharm/AHD	Prednisolone	19H19-B02-194548	1
Tianyao Pharma/Phönix	Prednisolone	1212021-01	1
Tianyao Pharma/Phönix	Prednisolone	NEPL110103	1

- 233 261 spectra from 1514 *Apo-Ident* customers from a total of 48 783 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Prednisolone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prednisolone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	1162	14	151 786
Type B	0	852	0	201 232
Type C	0	2760	46	233 261

The substance/substance group *Prednisolone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	98.8095 % (> 98.5544 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2958 %)
Type C	100.0000 % (> 99.9007 %)	98.3607 % (> 98.2537 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20773	21303	9.32	155.59
21303	21303	0.00	150.76
21449	21449	0.00	150.64
21604	21604	0.00	150.61
21660	21449	3.77	152.86
21849	21849	0.00	139.69
22435	22435	0.00	151.70
22467	22467	0.00	140.93
22651	21449	9.54	157.97
22709	22709	0.00	147.35
22783	22435	3.62	151.94
22803	22435	9.80	149.67
25192	25192	0.00	147.15
25688	25688	0.00	151.87

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Prednisolone acetate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20089-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Prednisolone acetate; Prednisoloni acetas

Special notes

When selecting the *Prednisolone acetate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Prednisolone acetate	9	13	420

Second-stage model

For differentiation of the substance/substance group *Prednisolone acetate* the following second-stage model is used:

- Submodel 08

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Prednisolone acetate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prednisone	73.25	50.42
⋮	⋮	⋮
Ephedrine hydrochloride	>50	146.64

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Prednisolone acetate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Prednisolone acetate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Prednisolone acetate	12091814	20784	80	20120416
Caelo	Prednisolone acetate	12324502	20877	40	20121112
Caelo	Prednisolone acetate	13262605	21448	60	20130923
Caelo	Prednisolone acetate	13262605	21450	60	20130923
Caelo	Prednisolone acetate	13262605	21450SI	47	20130923
Euro OTC	Prednisolone acetate	1306040	21096	40	20130812
Euro OTC	Prednisolone acetate	1209028-03	21530	60	AR-15-FG-010480-01
Euro OTC	Prednisolone acetate	1512020	22297	45	20160119*
Euro OTC	Prednisolone acetate	1512020	22297SI	44	20160119*
Euro OTC	Prednisolone acetate	2010016	25525	40	20210104*
Euro OTC	Prednisolone acetate	2010016	25525SI	40	20210104*
Fagron	Prednisolone acetate	12H14-N07	20795	40	20120829
Fagron	Prednisolone acetate	12H14-N07	20795SI	49	20120829
Fagron	Prednisolone acetate	15I23-B04-345785	24587	40	20151014

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 685 spectra of 14 reference samples from the substance/substance group *Prednisolone acetate*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 277 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1098 spectra of 28 reference samples from the substance/substance group *Prednisolone acetate*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Prednisolone acetate	180673	24534	40
Caelo	Prednisolone acetate	20001950	25215	40
Caelo	Prednisolone acetate	22001230	26129	30
Euro OTC	Prednisolone acetate	1607010	22710	40
Euro OTC	Prednisolone acetate	1701041	23142	40
Euro OTC	Prednisolone acetate	1805009	24133	40
Euro OTC	Prednisolone acetate	1903031	24636	40
Euro OTC	Prednisolone acetate	1911014	24960	40
Euro OTC	Prednisolone acetate	2201028	25954	40
Euro OTC	Prednisolone acetate	2309013	27008	30
Euro OTC	Prednisolone acetate	2410006	27459	30
Fagron	Prednisolone acetate	21K18-B05-220957	26169	40
Fagron	Prednisolone acetate	23G05-B13-228543	26916	40
Caelo	Prednisolone acetate	13262605	21448SI†	44
Caelo	Prednisolone acetate	180673	24534SI	80
Caelo	Prednisolone acetate	20001950	25215SI	40
Caelo	Prednisolone acetate	22001230	26129SI	40
Euro OTC	Prednisolone acetate	1607010	22710SI	40
Euro OTC	Prednisolone acetate	1701041	23142SI	24
Euro OTC	Prednisolone acetate	1805009	24133SI	40
Euro OTC	Prednisolone acetate	1903031	24636SI	40
Euro OTC	Prednisolone acetate	1911014	24960SI	40

continued on the next page

descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Prednisolone acetate	2201028	25954SI	40
Euro OTC	Prednisolone acetate	2309013	27008SI	40
Euro OTC	Prednisolone acetate	2410006	27459SI	30
Fagron	Prednisolone acetate	15I23-B04-345785	24587SI[†]	40
Fagron	Prednisolone acetate	21K18-B05-220957	26169SI	30
Fagron	Prednisolone acetate	23G05-B13-228543	26916SI	40

- 200 986 spectra from a total of 4030 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3573 spectra from 1047 *Apo-Ident* customers from 435 batches from the substance/substance group *Prednisolone acetate*.
- Among them are spectra of independent samples from 419 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Prednisolone acetate	15398303	1
	Prednisolone acetate	17086101	1
	Prednisolone acetate	21001844007	1
	Prednisolone acetate	21001844008	2
	Prednisolone acetate	21001844012	7
	Prednisolone acetate	22001230001	5
	Prednisolone acetate	22001230002	3
	Prednisolone acetate	22001230003	6
	Prednisolone acetate	22001230004	5
	Prednisolone acetate	22001230005	9
	Prednisolone acetate	22001230007	9
	Prednisolone acetate	22001230008	2
	Prednisolone acetate	22001230009	2
	Prednisolone acetate	2201028	2
	Prednisolone acetate	2201028-01	10
	Prednisolone acetate	2201028-02	11
	Prednisolone acetate	22I27-B10-223685	1
	Prednisolone acetate	230901301	1
	Prednisolone acetate	2309013-01	10
	Prednisolone acetate	B10-2236805	1
	Prednisolone acetate	B10-2237606	1
A.H. 23.05.13 ek: 5,40EUR	Prednisolone acetate	13A07-N07	1
A.H.D.	Prednisolone acetate	14175514	1
AHD 06.03.15	Prednisolone acetate	14175508	1
AHD 23.10.14 EK17,24	Prednisolone acetate	13262601	1
AHD/Euro	Prednisolone acetate	1805009-001	1
AHD	Prednisolone acetate	15055202	1
AHD	Prednisolone acetate	17086105	1
AHD	Prednisolone acetate	1903031-01	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
AHD	Prednisolone acetate	22001230001	1
AHD	Prednisolone acetate	22001230002	1
AHD	Prednisolone acetate	22001230003	3
AHD	Prednisolone acetate	22001230004	1
AHD	Prednisolone acetate	22001230007	1
Alliamce Healthcare	Prednisolone acetate	22001230001	1
Alliance Healthcare	Prednisolone acetate	12091807	1
Alliance Healthcare	Prednisolone acetate	1903031-02	1
Alliance Healthcare	Prednisolone acetate	1911014-02	2
Alliance Healthcare	Prednisolone acetate	20001950001	1
Alliance Healthcare	Prednisolone acetate	2010016-01	7
Alliance Healthcare	Prednisolone acetate	22001230007	1
Alliance Healthcare	Prednisolone acetate	2309013-01	4
Alliance	Prednisolone acetate	1209028-02	2
Alliance	Prednisolone acetate	22001230004	1
Alliance	Prednisolone acetate	K07A20190507	1
AllianceHealthcare	Prednisolone acetate	15055201	1
Allianz Healthcare	Prednisolone acetate	18067310	1
Anuh Pharma	Prednisolone acetate	21001844006	1
ANZAG	Prednisolone acetate	12091802	2
Anzag	Prednisolone acetate	13A07N07	1
Anzag	Prednisolone acetate	16246812	1
Anzag	Prednisolone acetate	192969005	1
apo-ident/Noweda	Prednisolone acetate	2010016-01	1
apo-ident/Phoenix	Prednisolone acetate	190272002	1
apo-ident	Prednisolone acetate	1512020-01	1
apo-ident	Prednisolone acetate	1805009-02	1
apomix	Prednisolone acetate	16246804	1
Avik Pharmaceutical ...	Prednisolone acetate	19C28-B02-361964	1
Beiersdorf AG	Prednisolone acetate	15055201	1
Beiersdorf AG	Prednisolone acetate	15398302	1
Bombastus	Prednisolone acetate	17185601	1
Bombastus	Prednisolone acetate	2255	1
cae	Prednisolone acetate	21001844004	1
Caeasar/Loretz,Fa.Gehe	Prednisolone acetate	14380910	1
Cael Sanacorp 05.02.2016	Prednisolone acetate	14175509	1
Cael Sanacorp 05.02.2016	Prednisolone acetate	14380901	1
Caeleo/ Kehr	Prednisolone acetate	21001844002	1
Caelo	Prednisolone acetate		5
Caelo	Prednisolone acetate	11080403	1
Caelo	Prednisolone acetate	11158002	1
Caelo	Prednisolone acetate	11158003	1
Caelo	Prednisolone acetate	11L21-N03	1
Caelo	Prednisolone acetate	12001844003	1
Caelo	Prednisolone acetate	1209028-02	2
Caelo	Prednisolone acetate	12091802	6
Caelo	Prednisolone acetate	12091803	3
Caelo	Prednisolone acetate	12091804	8
Caelo	Prednisolone acetate	12091806	3
Caelo	Prednisolone acetate	12091807	5
Caelo	Prednisolone acetate	12091808	5
Caelo	Prednisolone acetate	12091810	2
Caelo	Prednisolone acetate	12091813	1
Caelo	Prednisolone acetate	12091814	7
Caelo	Prednisolone acetate	12091815	2
Caelo	Prednisolone acetate	12324502	13
Caelo	Prednisolone acetate	12324503	1
Caelo	Prednisolone acetate	12324504	6
Caelo	Prednisolone acetate	12324505	16
Caelo	Prednisolone acetate	12324506	11

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednisolone acetate	12324508	9
Caelo	Prednisolone acetate	12324509	2
Caelo	Prednisolone acetate	12324514	5
Caelo	Prednisolone acetate	1234506	1
Caelo	Prednisolone acetate	12L05-N01	1
Caelo	Prednisolone acetate	1306040-01	1
Caelo	Prednisolone acetate	1306040-02	1
Caelo	Prednisolone acetate	13121715	1
Caelo	Prednisolone acetate	13262601	17
Caelo	Prednisolone acetate	13262602	8
Caelo	Prednisolone acetate	13262603	8
Caelo	Prednisolone acetate	13262605	13
Caelo	Prednisolone acetate	13262606	4
Caelo	Prednisolone acetate	13262609	4
Caelo	Prednisolone acetate	13343112	1
Caelo	Prednisolone acetate	1406014-01	2
Caelo	Prednisolone acetate	1406014-02	2
Caelo	Prednisolone acetate	14175508	16
Caelo	Prednisolone acetate	14175509	9
Caelo	Prednisolone acetate	14175512	1
Caelo	Prednisolone acetate	14175513	10
Caelo	Prednisolone acetate	14175514	7
Caelo	Prednisolone acetate	14380302	1
Caelo	Prednisolone acetate	14380901	19
Caelo	Prednisolone acetate	14380902	14
Caelo	Prednisolone acetate	14380903	2
Caelo	Prednisolone acetate	14380904	2
Caelo	Prednisolone acetate	14380905	21
Caelo	Prednisolone acetate	14380909	14
Caelo	Prednisolone acetate	14380910	10
Caelo	Prednisolone acetate	1475509	1
Caelo	Prednisolone acetate	1480905	1
Caelo	Prednisolone acetate	15055201	9
Caelo	Prednisolone acetate	15055202	16
Caelo	Prednisolone acetate	15055203	2
Caelo	Prednisolone acetate	15055206	10
Caelo	Prednisolone acetate	151202001	1
Caelo	Prednisolone acetate	1512020-01	4
Caelo	Prednisolone acetate	1523-B04-336299	1
Caelo	Prednisolone acetate	15298401	1
Caelo	Prednisolone acetate	15344002	1
Caelo	Prednisolone acetate	15396304	1
Caelo	Prednisolone acetate	15398302	14
Caelo	Prednisolone acetate	15398303	10
Caelo	Prednisolone acetate	15398304	8
Caelo	Prednisolone acetate	15398306	6
Caelo	Prednisolone acetate	15398307	10
Caelo	Prednisolone acetate	15398401	12
Caelo	Prednisolone acetate	15398402	15
Caelo	Prednisolone acetate	15398407	10
Caelo	Prednisolone acetate	15398408	11
Caelo	Prednisolone acetate	15B03B05302564	1
Caelo	Prednisolone acetate	15B03-B05-302564	2
Caelo	Prednisolone acetate	16/AKD2	1
Caelo	Prednisolone acetate	160701001	3
Caelo	Prednisolone acetate	1607010-01	6
Caelo	Prednisolone acetate	1616I-02106	1
Caelo	Prednisolone acetate	162446808	1
Caelo	Prednisolone acetate	162468	2
Caelo	Prednisolone acetate	16246801	17

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednisolone acetate	16246802	12
Caelo	Prednisolone acetate	16246803	20
Caelo	Prednisolone acetate	16246803-14317/1	1
Caelo	Prednisolone acetate	16246803-70317/1	1
Caelo	Prednisolone acetate	16246804	14
Caelo	Prednisolone acetate	16246805	2
Caelo	Prednisolone acetate	16246806	15
Caelo	Prednisolone acetate	16246807	18
Caelo	Prednisolone acetate	16246808	15
Caelo	Prednisolone acetate	16246809	3
Caelo	Prednisolone acetate	16246811	8
Caelo	Prednisolone acetate	16246812	11
Caelo	Prednisolone acetate	1624801	1
Caelo	Prednisolone acetate	1624806	1
Caelo	Prednisolone acetate	16248808	1
Caelo	Prednisolone acetate	165246802	1
Caelo	Prednisolone acetate	170104-01	1
Caelo	Prednisolone acetate	170104101	2
Caelo	Prednisolone acetate	1701041-01	5
Caelo	Prednisolone acetate	1701041-02	4
Caelo	Prednisolone acetate	17041802	1
Caelo	Prednisolone acetate	17086101	25
Caelo	Prednisolone acetate	170861015494	1
Caelo	Prednisolone acetate	17086102	12
Caelo	Prednisolone acetate	17086103	19
Caelo	Prednisolone acetate	17086103/1110917	1
Caelo	Prednisolone acetate	17086104	26
Caelo	Prednisolone acetate	17086105	26
Caelo	Prednisolone acetate	17086106	2
Caelo	Prednisolone acetate	17185601	30
Caelo	Prednisolone acetate	171856010	1
Caelo	Prednisolone acetate	17185602	29
Caelo	Prednisolone acetate	17185603	30
Caelo	Prednisolone acetate	17185604	4
Caelo	Prednisolone acetate	17401041-02	1
Caelo	Prednisolone acetate	1786103	1
Caelo	Prednisolone acetate	18004401	28
Caelo	Prednisolone acetate	18004402	22
Caelo	Prednisolone acetate	18004403	3
Caelo	Prednisolone acetate	18004903	1
Caelo	Prednisolone acetate	1805009	1
Caelo	Prednisolone acetate	180500901	1
Caelo	Prednisolone acetate	1805009-01	6
Caelo	Prednisolone acetate	1805009-02	2
Caelo	Prednisolone acetate	180500903	1
Caelo	Prednisolone acetate	1805009-03	1
Caelo	Prednisolone acetate	18067301	4
Caelo	Prednisolone acetate	18067302	24
Caelo	Prednisolone acetate	180673025724	1
Caelo	Prednisolone acetate	18067303	28
Caelo	Prednisolone acetate	18067307	38
Caelo	Prednisolone acetate	18067308	3
Caelo	Prednisolone acetate	18067309	36
Caelo	Prednisolone acetate	18067309P-190226-2	1
Caelo	Prednisolone acetate	18067309-P20180115Ma	1
Caelo	Prednisolone acetate	18067310	30
Caelo	Prednisolone acetate	18067313	1
Caelo	Prednisolone acetate	18067314	30
Caelo	Prednisolone acetate	18067314P-191022-8	1
Caelo	Prednisolone acetate	18067316	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednisolone acetate	18067317	21
Caelo	Prednisolone acetate	18067320	48
Caelo	Prednisolone acetate	18067323	2
Caelo	Prednisolone acetate	18067324	28
Caelo	Prednisolone acetate	18067324-B04	1
Caelo	Prednisolone acetate	18067325	6
Caelo	Prednisolone acetate	18398303	1
Caelo	Prednisolone acetate	1867309	1
Caelo	Prednisolone acetate	1867314	1
Caelo	Prednisolone acetate	19010303	1
Caelo	Prednisolone acetate	1903031-01	3
Caelo	Prednisolone acetate	1911014-01	1
Caelo	Prednisolone acetate	1911014-02	3
Caelo	Prednisolone acetate	19269004	2
Caelo	Prednisolone acetate	192969003	33
Caelo	Prednisolone acetate	192969004	35
Caelo	Prednisolone acetate	192969004P-200220-2	1
Caelo	Prednisolone acetate	192969005	38
Caelo	Prednisolone acetate	19J08-F02-365546	1
Caelo	Prednisolone acetate	19J0B-F02-366051	1
Caelo	Prednisolone acetate	2000019500002	1
Caelo	Prednisolone acetate	20001950001	12
Caelo	Prednisolone acetate	200019500010	1
Caelo	Prednisolone acetate	20001950002	18
Caelo	Prednisolone acetate	20001950003	12
Caelo	Prednisolone acetate	20001950004	13
Caelo	Prednisolone acetate	2000195001	1
Caelo	Prednisolone acetate	2000195004	1
Caelo	Prednisolone acetate	200019550002	1
Caelo	Prednisolone acetate	200034843003	1
Caelo	Prednisolone acetate	20003817016	1
Caelo	Prednisolone acetate	20003843001	32
Caelo	Prednisolone acetate	20003843003	43
Caelo	Prednisolone acetate	2000384300301972024	1
Caelo	Prednisolone acetate	20003843004	21
Caelo	Prednisolone acetate	200038443001	1
Caelo	Prednisolone acetate	200038443003	1
Caelo	Prednisolone acetate	20160727Ma1	1
Caelo	Prednisolone acetate	21001844001	1
Caelo	Prednisolone acetate	21001844002	23
Caelo	Prednisolone acetate	21001844003	22
Caelo	Prednisolone acetate	21001844004	15
Caelo	Prednisolone acetate	21001844006	12
Caelo	Prednisolone acetate	21001844006/221228	1
Caelo	Prednisolone acetate	21001844007	18
Caelo	Prednisolone acetate	21001844008	10
Caelo	Prednisolone acetate	21001844010	5
Caelo	Prednisolone acetate	21001844012	1
Caelo	Prednisolone acetate	21001844013	1
Caelo	Prednisolone acetate	2100184402	1
Caelo	Prednisolone acetate	2100184404	1
Caelo	Prednisolone acetate	2101844002	1
Caelo	Prednisolone acetate	21071808	1
Caelo	Prednisolone acetate	22001230001	7
Caelo	Prednisolone acetate	22001230002	7
Caelo	Prednisolone acetate	22001230003	6
Caelo	Prednisolone acetate	22001230004	1
Caelo	Prednisolone acetate	2200123001	1
Caelo	Prednisolone acetate	2200123002	1
Caelo	Prednisolone acetate	23051812	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Prednisolone acetate	26011905	1
Caelo	Prednisolone acetate	27051301	1
Caelo	Prednisolone acetate	313I-02106	1
Caelo	Prednisolone acetate	32304	1
Caelo	Prednisolone acetate	32304015	1
Caelo	Prednisolone acetate	4313A-02106	1
Caelo	Prednisolone acetate	5031511	1
Caelo	Prednisolone acetate	5398304	1
Caelo	Prednisolone acetate	6021306	1
Caelo	Prednisolone acetate	717Q-02106	1
Caelo	Prednisolone acetate	8067320	1
Caelo	Prednisolone acetate	80673201	1
Caelo	Prednisolone acetate	8699	1
Caelo	Prednisolone acetate	F02-3660501	1
Caeol/Noweda	Prednisolone acetate	16246802	1
Caesar & Lorenz GmbH	Prednisolone acetate	21001844006	1
Caesar & Loretz GmbH...	Prednisolone acetate	18067310	1
Caesar & Loretz GmbH...	Prednisolone acetate	17185603	1
Caesar & Loretz GmbH...	Prednisolone acetate	20001950003	1
Caesar & Loretz GmbH...	Prednisolone acetate	21001844008	1
Caesar & Loretz GmbH...	Prednisolone acetate	192969003	1
Caesar & Loretz GmbH...	Prednisolone acetate	192969003	1
Caesar & Loretz GmbH...	Prednisolone acetate	17086105	1
Caesar & Loretz GmbH...	Prednisolone acetate	17185601	1
Caesar & Loretz GmbH...	Prednisolone acetate	20003843003	1
Caesar & Loretz GmbH...	Prednisolone acetate	20001950001	1
Caesar & Loretz GmbH...	Prednisolone acetate	20003843004	3
Caesar & Loretz GmbH...	Prednisolone acetate	21000607004	1
Caesar & Loretz GmbH...	Prednisolone acetate	20003843001	1
Caesar & Loretz GmbH/E	Prednisolone acetate	192969005	1
Caesar & Loretz GmbH...	Prednisolone acetate	18067320	1
Caesar & Loretz GmbH...	Prednisolone acetate	192969005	1
Caesar & Loretz GmbH...	Prednisolone acetate	20003843003	1
Caesar & Loretz GmbH/Gehe	Prednisolone acetate	18067324	1
Caesar & Loretz GmbH/Gehe	Prednisolone acetate	192969003	1
Caesar & Loretz GmbH/Gehe	Prednisolone acetate	21001844002	1
Caesar & Loretz GmbH/Gehe	Prednisolone acetate	21001844007	1
Caesar & Loretz GmbH...	Prednisolone acetate	20001950004	2
Caesar & Loretz GmbH...	Prednisolone acetate	22001230001	1
Caesar & Loretz GmbH...	Prednisolone acetate	18067320	1
Caesar & Loretz GmbH...	Prednisolone acetate	192969004	1
Caesar & Loretz GmbH...	Prednisolone acetate	20003843001	1
Caesar & Loretz GmbH/Kehr	Prednisolone acetate	192969004	1
Caesar & Loretz GmbH...	Prednisolone acetate	18067320	1
Caesar & Loretz GmbH...	Prednisolone acetate	20C06-F02-3700407	1
Caesar & Loretz GmbH...	Prednisolone acetate	F12-3742909	1
Caesar & Loretz GmbH/Ph	Prednisolone acetate	192969005	1
Caesar & Loretz GmbH...	Prednisolone acetate	22001230001	3
Caesar & Loretz GmbH...	Prednisolone acetate	1911014-02	1
Caesar & Loretz GmbH...	Prednisolone acetate	192969005	1
Caesar & Loretz GmbH...	Prednisolone acetate	20001950004	1
Caesar & Loretz GmbH...	Prednisolone acetate	20003843003	1
Caesar & Loretz GmbH...	Prednisolone acetate	21001844003	2
Caesar & Loretz GmbH...	Prednisolone acetate	21001844008	1
Caesar & Loretz GmbH...	Prednisolone acetate	22001230001	1
Caesar & Loretz GmbH...	Prednisolone acetate	22001230004	1
Caesar & Loretz GmbH...	Prednisolone acetate	22001230002	1
Caesar & Loretz GmbH	Prednisolone acetate	17185603	1
Caesar & Loretz GmbH	Prednisolone acetate	180667317	1
Caesar & Loretz GmbH	Prednisolone acetate	18067303	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Prednisolone acetate	18067307	5
Caesar & Loretz GmbH	Prednisolone acetate	18067309	2
Caesar & Loretz GmbH	Prednisolone acetate	18067310	10
Caesar & Loretz GmbH	Prednisolone acetate	18067314	7
Caesar & Loretz GmbH	Prednisolone acetate	18067317	9
Caesar & Loretz GmbH	Prednisolone acetate	18067320	3
Caesar & Loretz GmbH	Prednisolone acetate	18067323	1
Caesar & Loretz GmbH	Prednisolone acetate	18067324	1
Caesar & Loretz GmbH	Prednisolone acetate	18067325	1
Caesar & Loretz GmbH	Prednisolone acetate	1903031-01	1
Caesar & Loretz GmbH	Prednisolone acetate	192969002	1
Caesar & Loretz GmbH	Prednisolone acetate	192969003	5
Caesar & Loretz GmbH	Prednisolone acetate	192969004	8
Caesar & Loretz GmbH	Prednisolone acetate	192969005	15
Caesar & Loretz GmbH	Prednisolone acetate	20001950001	11
Caesar & Loretz GmbH	Prednisolone acetate	20001950002	9
Caesar & Loretz GmbH	Prednisolone acetate	20001950003	9
Caesar & Loretz GmbH	Prednisolone acetate	20001950004	8
Caesar & Loretz GmbH	Prednisolone acetate	20001950005	3
Caesar & Loretz GmbH	Prednisolone acetate	20003843001	11
Caesar & Loretz GmbH	Prednisolone acetate	20003843002	1
Caesar & Loretz GmbH	Prednisolone acetate	20003843003	13
Caesar & Loretz GmbH	Prednisolone acetate	20003843004	9
Caesar & Loretz GmbH	Prednisolone acetate	2001950002	1
Caesar & Loretz GmbH	Prednisolone acetate	21001844002	6
Caesar & Loretz GmbH	Prednisolone acetate	21001844003	10
Caesar & Loretz GmbH	Prednisolone acetate	21001844004	9
Caesar & Loretz GmbH	Prednisolone acetate	21001844006	4
Caesar & Loretz GmbH	Prednisolone acetate	21001844007	1
Caesar & Loretz GmbH	Prednisolone acetate	21001844008	5
Caesar & Loretz GmbH	Prednisolone acetate	21001844010	2
Caesar & Loretz GmbH	Prednisolone acetate	22001230001	3
Caesar & Loretz GmbH	Prednisolone acetate	22001230003	1
Caesar & Loretz GmbH	Prednisolone acetate	22001230004	1
Caesar & Loretz Hild…	Prednisolone acetate	18067317	1
Caesar & Loretz/Geil…	Prednisolone acetate	18067320	1
Caesar / Ebert & Jacobi	Prednisolone acetate	17185603	1
Caesar Loretz	Prednisolone acetate	192969005	2
Caesar&Loretz GmbH,P…	Prednisolone acetate	17086103	2
Caesar&Loretz GmbH	Prednisolone acetate	15396408	1
Caesar&Loretz GmbH	Prednisolone acetate	18067324	1
Caesar&Loretz GmbH	Prednisolone acetate	20003843003	1
Caesar&Loretz GmbH	Prednisolone acetate	22001230002	1
Caesar&loretz,AHC,29…	Prednisolone acetate	15398306	1
Caesar&loretz,Phoeni…	Prednisolone acetate		1
Caesar&loretz,Phoenix	Prednisolone acetate	13262606	1
Caesar&loretz,Phoenix	Prednisolone acetate	14175513	1
Caesar&Loretz,Phönix…	Prednisolone acetate	15398302	1
caesar&loretz,Phönix	Prednisolone acetate	15055202	2
caesar&loretz	Prednisolone acetate	14380909	1
Caesar&Loretz	Prednisolone acetate	18067320	1
Caesar&LoretzGmbH,11…	Prednisolone acetate	16246803	1
Cealo/Gehe	Prednisolone acetate	20001950002	1
Cealo	Prednisolone acetate	14175513	1
cealo	Prednisolone acetate	18067303	1
Cealo	Prednisolone acetate	19296004	1
Cealo	Prednisolone acetate	192969005	1
Cealo	Prednisolone acetate	20001950001	1
Cealo	Prednisolone acetate	21001844004	1
Ceasar & Loretz GmbH…	Prednisolone acetate	18067303	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Delta	Prednisolone acetate	17086103	1
Delta	Prednisolone acetate	17185602	1
Delta	Prednisolone acetate	18067314	1
Ebert & Jacobi	Prednisolone acetate	15398307	1
EuRho / Fiebig	Prednisolone acetate	1903031-01	1
EuRho / Gehe	Prednisolone acetate	1903031-01	1
EuRho/Gehe	Prednisolone acetate	1805009-03	1
EuRho/Noweda	Prednisolone acetate	18004401	1
EuRho/Phönix	Prednisolone acetate	1805009-03	1
EuRho/Phönix	Prednisolone acetate	1903031-01	1
Eurho/Phönix	Prednisolone acetate	201001601	1
EuRho/Phönix	Prednisolone acetate	201001601	1
EuRho/Phönix	Prednisolone acetate	2010016-01	1
Eurho/Sanacorp	Prednisolone acetate	1805009-01	2
EuRho/Sanacorp	Prednisolone acetate	1903031-01	3
EuRho/Sanacorp	Prednisolone acetate	1911014-01	2
EuRho	Prednisolone acetate	1306040-03	1
EuRho	Prednisolone acetate	1406014-02	1
EuRho	Prednisolone acetate	1512020-01	1
Eurho	Prednisolone acetate	1701041-01	2
EuRho	Prednisolone acetate	1701041-01	1
EuRho	Prednisolone acetate	170104102	1
EuRho	Prednisolone acetate	1701041-02	1
EuRho	Prednisolone acetate	1805009-01	2
EuRho	Prednisolone acetate	1805009-02	1
EuRho	Prednisolone acetate	1911014-01	3
EuRho	Prednisolone acetate	1911014-02	1
EuRho	Prednisolone acetate	2010016-01	3
Euro OTC	Prednisolone acetate		1
Euro OTC	Prednisolone acetate	1/01041-01	1
Euro OTC	Prednisolone acetate	1108043-01	2
Euro OTC	Prednisolone acetate	1108043-02	13
Euro OTC	Prednisolone acetate	1203028-03	1
Euro OTC	Prednisolone acetate	1209028	1
Euro OTC	Prednisolone acetate	1209028-01	3
Euro OTC	Prednisolone acetate	1209028-02	11
Euro OTC	Prednisolone acetate	1209028-03	2
Euro OTC	Prednisolone acetate	1305009-01	1
Euro OTC	Prednisolone acetate	1306010-01	1
Euro OTC	Prednisolone acetate	1306040-01	22
Euro OTC	Prednisolone acetate	130604002	1
Euro OTC	Prednisolone acetate	1306040-02	14
Euro OTC	Prednisolone acetate	1306040-03	1
Euro OTC	Prednisolone acetate	1306040-1	1
Euro OTC	Prednisolone acetate	13262601	1
Euro OTC	Prednisolone acetate	13262606	1
Euro OTC	Prednisolone acetate	1406012-02	1
Euro OTC	Prednisolone acetate	1406014-01	17
Euro OTC	Prednisolone acetate	1406014-02	13
Euro OTC	Prednisolone acetate	1407010-01	1
Euro OTC	Prednisolone acetate	14406014-02	1
Euro OTC	Prednisolone acetate	1460614-01	1
Euro OTC	Prednisolone acetate	1501036	1
Euro OTC	Prednisolone acetate	150103601	3
Euro OTC	Prednisolone acetate	1501036-01	20
Euro OTC	Prednisolone acetate	150103602	1
Euro OTC	Prednisolone acetate	1501036-02	35
Euro OTC	Prednisolone acetate	151202001	1
Euro OTC	Prednisolone acetate	1512020-01	34
Euro OTC	Prednisolone acetate	1607010	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Prednisolone acetate	160701001	2
Euro OTC	Prednisolone acetate	1607010-01	98
Euro OTC	Prednisolone acetate	1607010-10	1
Euro OTC	Prednisolone acetate	161005PA	1
Euro OTC	Prednisolone acetate	16246801	2
Euro OTC	Prednisolone acetate	170104-02	1
Euro OTC	Prednisolone acetate	1701041	2
Euro OTC	Prednisolone acetate	170104101	3
Euro OTC	Prednisolone acetate	1701041-01	52
Euro OTC	Prednisolone acetate	170104102	1
Euro OTC	Prednisolone acetate	1701041-02	53
Euro OTC	Prednisolone acetate	1701041-03	8
Euro OTC	Prednisolone acetate	170413PA/1607010-01	1
Euro OTC	Prednisolone acetate	17086101	1
Euro OTC	Prednisolone acetate	18004403	1
Euro OTC	Prednisolone acetate	1805009	5
Euro OTC	Prednisolone acetate	1805009-01	57
Euro OTC	Prednisolone acetate	1805009-02	39
Euro OTC	Prednisolone acetate	1805009-03	14
Euro OTC	Prednisolone acetate	18050099-01	1
Euro OTC	Prednisolone acetate	180509-01	1
Euro OTC	Prednisolone acetate	180509-03	1
Euro OTC	Prednisolone acetate	18067302	1
Euro OTC	Prednisolone acetate	18067320	1
Euro OTC	Prednisolone acetate	1903031	6
Euro OTC	Prednisolone acetate	190303101	4
Euro OTC	Prednisolone acetate	1903031-01	92
Euro OTC	Prednisolone acetate	190303102	1
Euro OTC	Prednisolone acetate	1903031-02	27
Euro OTC	Prednisolone acetate	1911014	1
Euro OTC	Prednisolone acetate	191101401	3
Euro OTC	Prednisolone acetate	1911014-01	105
Euro OTC	Prednisolone acetate	191101402	1
Euro OTC	Prednisolone acetate	1911014-02	43
Euro OTC	Prednisolone acetate	1911014-03	1
Euro OTC	Prednisolone acetate	191104-01	1
Euro OTC	Prednisolone acetate	191104-02	1
Euro OTC	Prednisolone acetate	19111014	1
Euro OTC	Prednisolone acetate	2(1903031-01)	1
Euro OTC	Prednisolone acetate	200540	2
Euro OTC	Prednisolone acetate	2010010-01	1
Euro OTC	Prednisolone acetate	201001601	4
Euro OTC	Prednisolone acetate	2010016-01	94
Euro OTC	Prednisolone acetate	20-10016-01	1
Euro OTC	Prednisolone acetate	2201028	1
Euro OTC	Prednisolone acetate	2201028-01	39
Euro OTC	Prednisolone acetate	220128-01	1
Euro OTC	Prednisolone acetate	221028-01	1
Euro OTC	Prednisolone acetate	2215I-02106	1
Euro OTC	Prednisolone acetate	2413Q02106	1
Euro OTC	Prednisolone acetate	2507212106	1
Euro OTC	Prednisolone acetate	2517Q-02106	1
Euro OTC	Prednisolone acetate	2714U-02106	1
Euro OTC	Prednisolone acetate	289295	1
Euro OTC	Prednisolone acetate	2918E-02106	1
Euro OTC	Prednisolone acetate	5012I-02106	1
Euro OTC	Prednisolone acetate	514U2106	1
Euro OTC	Prednisolone acetate	711212106	1
Euro OTC	Prednisolone acetate	911014-021	1
Euro OTC	Prednisolone acetate	K07A20140304M	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Prednisolone acetate	K07A20170803M	1
Euro OTC	Prednisolone acetate	K07A20190507	7
Euro OTC	Prednisolone acetate	K07D20161003M	1
Euro OTC	Prednisolone acetate	P161	1
Euro/ Gehe	Prednisolone acetate	1911014-02	1
EUro/AHD	Prednisolone acetate	1306040-01	1
EUro/AHD	Prednisolone acetate	1306040-02	1
Euro/Phönix	Prednisolone acetate	1805009-02	1
Euro/Sana	Prednisolone acetate	1805009-01	1
Euro/Sanacorp	Prednisolone acetate	1805009-02	1
Euro/Sanacorp	Prednisolone acetate	1911014-01	2
Euro/Sanacorp	Prednisolone acetate	20J01-F12-374299	1
EuRoh/ Gehe	Prednisolone acetate	18004402	1
Euroo/Gehe	Prednisolone acetate	1501036-02	1
Fagro/Noweda	Prednisolone acetate	15I23-B04-345785	2
fagro	Prednisolone acetate	15B03-B05-302564	1
Fagron	Prednisolone acetate		3
Fagron	Prednisolone acetate	113Q-02106	1
Fagron	Prednisolone acetate	115B03-B05-308582	1
Fagron	Prednisolone acetate	11A31-N03	1
Fagron	Prednisolone acetate	11I09N-08	1
Fagron	Prednisolone acetate	11I09-N08	1
Fagron	Prednisolone acetate	12324502	1
Fagron	Prednisolone acetate	12C19-N03	4
Fagron	Prednisolone acetate	12C19-NO3	1
Fagron	Prednisolone acetate	12G25-N05	5
Fagron	Prednisolone acetate	12h14-n07	1
Fagron	Prednisolone acetate	12H14-N07	4
Fagron	Prednisolone acetate	12H14-NO7	1
Fagron	Prednisolone acetate	12J10/N05	1
Fagron	Prednisolone acetate	12J10-N05	1
Fagron	Prednisolone acetate	12k20-b04293971	1
Fagron	Prednisolone acetate	12L05-N01	5
Fagron	Prednisolone acetate	12L11-B04-286905	1
Fagron	Prednisolone acetate	12L11-B40	1
Fagron	Prednisolone acetate	12L11-B40-286905	13
Fagron	Prednisolone acetate	12L11-B40-286915	2
Fagron	Prednisolone acetate	13262605	1
Fagron	Prednisolone acetate	13a07n07	1
Fagron	Prednisolone acetate	13A07-N07	7
Fagron	Prednisolone acetate	13D03-N06	1
Fagron	Prednisolone acetate	13K20-B04-289494	2
Fagron	Prednisolone acetate	13K20-B04-289495	3
Fagron	Prednisolone acetate	13K20-B04-293970	1
Fagron	Prednisolone acetate	13K20-B04-293971	3
Fagron	Prednisolone acetate	14380909	1
Fagron	Prednisolone acetate	14D04-B03-299294	4
Fagron	Prednisolone acetate	14D04B03299295	1
Fagron	Prednisolone acetate	14G30-B13	2
Fagron	Prednisolone acetate	14G30-B13-299293	5
Fagron	Prednisolone acetate	14G30-B13-302562	1
Fagron	Prednisolone acetate	15/23-B04-334668	1
Fagron	Prednisolone acetate	15/23-B04-334688	1
Fagron	Prednisolone acetate	15/23-B04-334702	1
Fagron	Prednisolone acetate	15/23-B04-336299	1
Fagron	Prednisolone acetate	15/23-B04-341793	1
Fagron	Prednisolone acetate	15/23-B04-345785	1
Fagron	Prednisolone acetate	15055201	1
Fagron	Prednisolone acetate	1523-B04	1
Fagron	Prednisolone acetate	1523-b04-345785	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednisolone acetate	15-23-B04-346700	1
Fagron	Prednisolone acetate	15398401	1
Fagron	Prednisolone acetate	15803-B05	1
Fagron	Prednisolone acetate	15B03_B05_302564	2
Fagron	Prednisolone acetate	15B03-B05	3
Fagron	Prednisolone acetate	15b03-b05-302564	1
Fagron	Prednisolone acetate	15B03B05302564	1
Fagron	Prednisolone acetate	15B03-B05-302564	17
Fagron	Prednisolone acetate	15B03-B05-302566	3
Fagron	Prednisolone acetate	15B03-B05-308574	2
Fagron	Prednisolone acetate	15B03-B05-308582	7
Fagron	Prednisolone acetate	15B03-B05-302564	1
Fagron	Prednisolone acetate	15F29-B07-317179	4
Fagron	Prednisolone acetate	15F29-B07-321001	2
Fagron	Prednisolone acetate	15F29-B07-323268	2
Fagron	Prednisolone acetate	15I23-B04	2
Fagron	Prednisolone acetate	15I23-B04-327929	1
Fagron	Prednisolone acetate	15I23-B04-331154	8
Fagron	Prednisolone acetate	15I23-B04-334688	1
Fagron	Prednisolone acetate	15I23-B04-334702	3
Fagron	Prednisolone acetate	15i23-b04-336299	1
Fagron	Prednisolone acetate	15I23-B04-336299	2
Fagron	Prednisolone acetate	15I23-B04-340335	1
Fagron	Prednisolone acetate	15I23-B04-341793	2
Fagron	Prednisolone acetate	15I23-B04-345785	2
Fagron	Prednisolone acetate	15I23-B04-346700	1
Fagron	Prednisolone acetate	1512351-b04-336299	1
Fagron	Prednisolone acetate	15123-B04-324088	1
Fagron	Prednisolone acetate	15123-B04-327929	1
Fagron	Prednisolone acetate	15123-B04-341793	1
Fagron	Prednisolone acetate	15123-B4-334688	1
Fagron	Prednisolone acetate	1607010-01	1
Fagron	Prednisolone acetate	17189601	1
Fagron	Prednisolone acetate	1805009-01	1
Fagron	Prednisolone acetate	180713a	1
Fagron	Prednisolone acetate	1911014-01	1
Fagron	Prednisolone acetate	19C28-B02-361965	1
Fagron	Prednisolone acetate	19J08	1
Fagron	Prednisolone acetate	19J08-F02	2
Fagron	Prednisolone acetate	19J08-F02-365546	1
Fagron	Prednisolone acetate	19J08-F02-366051	1
Fagron	Prednisolone acetate	200540-0013	1
Fagron	Prednisolone acetate	20C06-F02	3
Fagron	Prednisolone acetate	20C06-F02-370047	2
Fagron	Prednisolone acetate	20C06-F02-370049	4
Fagron	Prednisolone acetate	20J01-F12	1
Fagron	Prednisolone acetate	20J01-F12-374299	2
Fagron	Prednisolone acetate	20J01-F12-374300	3
Fagron	Prednisolone acetate	20J01-F12-374302	1
Fagron	Prednisolone acetate	20J02-F12	1
Fagron	Prednisolone acetate	21K18-B05-220957	3
Fagron	Prednisolone acetate	5444	1
Fagron	Prednisolone acetate	6082013D	1
Fagron	Prednisolone acetate	F02-3700409	1
Fagron	Prednisolone acetate	F12-3742909	1
Fagron	Prednisolone acetate	F12-374299	1
Fagron	Prednisolone acetate	F12-3743000	3
Fagron	Prednisolone acetate	K07A20130903M	1
Fagron	Prednisolone acetate	K07D20150105M	2
Fagron	Prednisolone acetate	K07D20150503M	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prednisolone acetate	pa/m/013/19	1
Fagron	Prednisolone acetate	PA/M/016/19	1
Fargo	Prednisolone acetate	12025-N05	1
Fargon	Prednisolone acetate	13A07-N07	1
Fiebig	Prednisolone acetate	1501036-01	1
Fiebig	Prednisolone acetate	18067303	1
Fiebig	Prednisolone acetate	18067307	1
Fiebig	Prednisolone acetate	18067317	1
Finteler Apotheke	Prednisolone acetate	16246812	1
Finteler Apotheke	Prednisolone acetate	17086103	1
Fragron	Prednisolone acetate	K07A20131101M	1
Gehe / EuRho	Prednisolone acetate	1911014-02	1
GEHE 03.07.2014	Prednisolone acetate	13262605	1
Gehe amax	Prednisolone acetate	17086101	2
Gehe amax	Prednisolone acetate	1911014-01	1
Gehe Rostock	Prednisolone acetate	2201028	1
Gehe/Apo-Ident	Prednisolone acetate	1701041-02	2
Gehe/EuRho 10.09.2021	Prednisolone acetate	2010016-01	2
Gehe/EuRo	Prednisolone acetate	1701041-02	1
Gehe/EuRoh	Prednisolone acetate	191101402	1
Gehe	Prednisolone acetate	1209028-01	1
Gehe	Prednisolone acetate	1209028-02	2
Gehe	Prednisolone acetate	12H14-N07	1
Gehe	Prednisolone acetate	13262609	1
Gehe	Prednisolone acetate	1406014-01	1
Gehe	Prednisolone acetate	1501036-02	2
Gehe	Prednisolone acetate	1512020-01	1
Gehe	Prednisolone acetate	15B03-B05-302566	1
Gehe	Prednisolone acetate	15I23-B04-327929	1
Gehe	Prednisolone acetate	160701001	1
Gehe	Prednisolone acetate	1607010-01	1
Gehe	Prednisolone acetate	16246803	2
Gehe	Prednisolone acetate	16246806	2
GEHE	Prednisolone acetate	16246807	1
Gehe	Prednisolone acetate	16246812	1
Gehe	Prednisolone acetate	1701041-01	2
Gehe	Prednisolone acetate	1701041-02	2
Gehe	Prednisolone acetate	17185601	1
GEHE	Prednisolone acetate	17185601	1
Gehe	Prednisolone acetate	17185602	2
Gehe	Prednisolone acetate	1805009-01	1
Gehe	Prednisolone acetate	1805009-03	1
GEHE	Prednisolone acetate	18067302	1
Gehe	Prednisolone acetate	18067303	2
Gehe	Prednisolone acetate	18067309	1
Gehe	Prednisolone acetate	18067310	1
Gehe	Prednisolone acetate	18067314	2
Gehe	Prednisolone acetate	1903031-01	1
GEHE	Prednisolone acetate	1903031-01	1
Gehe	Prednisolone acetate	1911014-01	2
Gehe	Prednisolone acetate	192969004	1
Gehe	Prednisolone acetate	2010016-01	2
Gehe	Prednisolone acetate	2201028-01	2
Gehe	Prednisolone acetate	2201028-02	1
Hanan/Phoenix	Prednisolone acetate	K07A20180303M	1
Henan / Gehe	Prednisolone acetate	20001950002	2
Henan Lihua Pharm/AHD	Prednisolone acetate	18067310	1
Henan Lihua Pharmace…	Prednisolone acetate	14G30-B13	1
Henan Lihua Pharmace…	Prednisolone acetate	1903031-01	1
Henan Lihua Pharmace…	Prednisolone acetate	2010016-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Henan Lihua/Phönix	Prednisolone acetate	1911014-02	1
Henan Lihus Pharm. C...	Prednisolone acetate	1903031-0	1
Henan Lihus Pharm. C...	Prednisolone acetate	1911014-02	1
Henan LP / Gehe	Prednisolone acetate	192969005	1
Henan/Alliance	Prednisolone acetate	18067314	1
Henan/Noweda	Prednisolone acetate	K07A20170803M	1
Henan/Noweda	Prednisolone acetate	K07A20190507	2
Henan/Phoenix	Prednisolone acetate	K07A20180603M	2
Kehr	Prednisolone acetate	1406014-01	1
L30	Prednisolone acetate	18004402	1
L30	Prednisolone acetate	18067303	1
Lihua Pharm	Prednisolone acetate	K07A20140302M	1
Lihua Pharma	Prednisolone acetate	1406014-01	1
Max Jenne/Euro	Prednisolone acetate	1911014-01	1
Nachprüfung	Prednisolone acetate	1019I-02106	1
Nachprüfung	Prednisolone acetate	2082019-2	1
NMoweda	Prednisolone acetate	2201028-01	1
Noweda 13.11. EK 17,81	Prednisolone acetate	ko7A20200901	2
Noweda 18.05.2015	Prednisolone acetate	14D04-B03-299294	1
Noweda Taucha	Prednisolone acetate	190303101	1
Noweda/EuRo	Prednisolone acetate	1607010-01	1
Noweda	Prednisolone acetate	1209028-01	1
Noweda	Prednisolone acetate	12324506	1
Noweda	Prednisolone acetate	12L11-B40-286905	1
noweda	Prednisolone acetate	14175513	1
Noweda	Prednisolone acetate	15055202	1
Noweda	Prednisolone acetate	1523-B04-334688	1
Noweda	Prednisolone acetate	15398303	1
Noweda	Prednisolone acetate	1701041-02	1
Noweda	Prednisolone acetate	17010410203707556	1
Noweda	Prednisolone acetate	17185602	1
Noweda	Prednisolone acetate	1805009-01	1
Noweda	Prednisolone acetate	18067302	1
Noweda	Prednisolone acetate	18067325	1
Noweda	Prednisolone acetate	1903031-01	2
Noweda	Prednisolone acetate	1903301_01	1
Noweda	Prednisolone acetate	191101401	1
Noweda	Prednisolone acetate	1911014-01	5
Noweda	Prednisolone acetate	1911014-02	3
Noweda	Prednisolone acetate	192969003	1
Noweda	Prednisolone acetate	19J08-F02-366051	1
Noweda	Prednisolone acetate	2010016-01	2
Noweda	Prednisolone acetate	22001230004	1
Noweda	Prednisolone acetate	22001230007	1
Noweda	Prednisolone acetate	2201028	1
Noweda	Prednisolone acetate	2201028-02	2
Noweda	Prednisolone acetate	230901301	1
Noweda	Prednisolone acetate	K07D20150105M	1
Phoenix	Prednisolone acetate	12L11-B40-286905	1
Phoenix	Prednisolone acetate	14380905	1
Phoenix	Prednisolone acetate	17185601	1
Phoenix	Prednisolone acetate	17185602	2
Phoenix	Prednisolone acetate	18067310	1
Phoenix	Prednisolone acetate	18067314	2
Phoenix	Prednisolone acetate	1911014-01	1
Phoenix	Prednisolone acetate	1911014-02	1
Phoenix	Prednisolone acetate	192969004	2
Phoenix	Prednisolone acetate	20001950001	1
Phoenix	Prednisolone acetate	20003843003	1
Phoenix	Prednisolone acetate	200540	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Prednisolone acetate	2010016-01	1
Phoenix	Prednisolone acetate	2010016-1	1
Phoenix	Prednisolone acetate	21001844002	1
Phoenix	Prednisolone acetate	22001230003	1
Phoenix	Prednisolone acetate	2200123004	1
Phoenix	Prednisolone acetate	3369	1
Phönix 09.05.2019	Prednisolone acetate	1805009-02	1
Phönix 23.08.2019	Prednisolone acetate	18067320	1
Phönix Gotha	Prednisolone acetate	18067310	1
Phönix Gotha	Prednisolone acetate	18067314	1
Phönix W.E:17.03.18 ...	Prednisolone acetate	17185601	1
Phönix, Avik Pharmac...	Prednisolone acetate	19J08-F02-365543	1
Phönix	Prednisolone acetate	11158008	1
Phönix	Prednisolone acetate	1209028-02	1
Phönix	Prednisolone acetate	12324506	1
Phönix	Prednisolone acetate	13262605	2
phönix	Prednisolone acetate	14380902	2
phönix	Prednisolone acetate	14380910	1
phönix	Prednisolone acetate	1438910	1
phönix	Prednisolone acetate	1512020-01	1
phönix	Prednisolone acetate	15398303	1
Phönix	Prednisolone acetate	15398303	1
phönix	Prednisolone acetate	15398402	1
phönix	Prednisolone acetate	16246803	3
Phönix	Prednisolone acetate	16246804	1
phönix	Prednisolone acetate	16246806	1
phönix	Prednisolone acetate	16246807	1
Phönix	Prednisolone acetate	17185602	2
Phönix	Prednisolone acetate	17185603	1
Phönix	Prednisolone acetate	1805009-01	1
Phönix	Prednisolone acetate	18067303	3
Phönix	Prednisolone acetate	18067317	1
Phönix	Prednisolone acetate	18067320	1
Phönix	Prednisolone acetate	1903031-01	1
Phönix	Prednisolone acetate	192969004	1
Phönix	Prednisolone acetate	192969005	2
Phönix	Prednisolone acetate	20001950001	1
Phönix	Prednisolone acetate	20003843003	1
Phönix	Prednisolone acetate	2001950001	1
Phönix	Prednisolone acetate	21001844002	2
Phönix	Prednisolone acetate	2200001230007	1
Phönix_28.11.2018	Prednisolone acetate	1805009-01	2
PhönixWE:10.02.2017 ...	Prednisolone acetate	16246806	1
Post Apotheke	Prednisolone acetate	18067301	1
Röntgen	Prednisolone acetate	1911014-02	1
Röntgen	Prednisolone acetate	192969004	1
Sana	Prednisolone acetate	15L23B04345785	1
Sanacorp 07.06.2019 ...	Prednisolone acetate	18067307	1
Sanacorp 14.03.2017 ...	Prednisolone acetate	16246802	1
Sanacorp	Prednisolone acetate	12091808	1
sanacorp	Prednisolone acetate	14380909	1
Sanacorp	Prednisolone acetate	15055206	1
Sanacorp	Prednisolone acetate	15398408	1
Sanacorp	Prednisolone acetate	15123-B04-334688	2
Sanacorp	Prednisolone acetate	15123-B04-341793	1
Sanacorp	Prednisolone acetate	17086104	1
Sanacorp	Prednisolone acetate	17185601	1
Sanacorp	Prednisolone acetate	17185602	1
Sanacorp	Prednisolone acetate	17185603	1
Sanacorp	Prednisolone acetate	18067303	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Prednisolone acetate	18067307	1
Sanacorp	Prednisolone acetate	18067309	2
Sanacorp	Prednisolone acetate	19003031-01	1
Sanacorp	Prednisolone acetate	1911014-01	1
sanacorp	Prednisolone acetate	19J08-F02-365542	1
sanacorp	Prednisolone acetate	200607	1
Sanacorp	Prednisolone acetate	20J01-F12-3743000	1
Sanacorp	Prednisolone acetate	21001844012	1
Sanacorp	Prednisolone acetate	22001230001	1
Sanacorp	Prednisolone acetate	22001230002	1
Sanacorp	Prednisolone acetate	22001230003	1
Sanacorp	Prednisolone acetate	2201028-01	1
Sanacorp	Prednisolone acetate	K07A20200902	1
Sanofi / Gehe	Prednisolone acetate	16246801	1
Spangro 08.05.2018	Prednisolone acetate	17185601	1
Spangro 30.5.14	Prednisolone acetate	13262606	1
Symbiotica Spec./Phönix	Prednisolone acetate	1306040-02	1
Symbiotika/Anzag	Prednisolone acetate	1306040-01	1
VDL;7,15EUR, 21:06:14	Prednisolone acetate	13262602	1
Wolf-Apotheke	Prednisolone acetate	14380911	1

- 232 494 spectra from 1514 *Apo-Ident* customers from a total of 48 836 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Prednisolone acetate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prednisolone acetate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	685	0	152 277
Type B	0	1098	0	200 986
Type C	0	3561	12	232 494

The substance/substance group *Prednisolone acetate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1241 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4536 %)
Type C	100.0000 % (> 99.9007 %)	99.6641 % (> 99.5802 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20784	22297	8.81	86.59
20795	22297	9.70	79.19
20877	22297	10.77	84.72
21096	21530	5.85	80.88
21448	22297	7.36	82.87
21450	22297	7.26	81.58
21530	21530	0.00	78.70
22297	22297	0.00	83.84
24587	22297	14.34	77.16
25525	25525	0.00	79.38

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Prednisolone hydrogen succinate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20838-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Prednisolone hydrogen succinate; Prednisoloni hydrogenosuccinas

Special notes

When selecting the *Prednisolone hydrogen succinate* substance/substance group, the following information is displayed to the user:

- Advice: Currently no longer available from major pharmaceutical manufacturers. Therefore, batch maintenance is currently not possible.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Prednisolone hydrogen succinate	3	2	10

Second-stage model

For differentiation of the substance/substance group *Prednisolone hydrogen succinate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Prednisolone hydrogen succinate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Estriol	80.66	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Prednisolone hydrogen succinate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Prednisolone hydrogen succinate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Prednisolone hydrogen suc…	2011003	25644	40	20201223*
Fagron	Prednisolone hydrogen suc…	13D16-N11	20956	40	1509250
Fagron	Prednisolone hydrogen suc…	14G29-B07-304733	22652	40	1701370
Fagron	Prednisolone hydrogen suc…	14G29-B07-304733	22723	40	20140825

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 160 spectra of 4 reference samples from the substance/substance group *Prednisolone hydrogen succinate*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 802 spectra from a total of 2839 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Prednisolone hydrogen succinate*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Prednisolone hydrogen suc…	12A20-N11	20838	40
Fagron	Prednisolone hydrogen suc…	15C11-B05-344778	24058	40

- 202 004 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 16 spectra from 12 *Apo-Ident* customers from 11 batches from the substance/substance group *Prednisolone hydrogen succinate*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Prednisolone hydrogen suc…	12A20-N11	1
Caelo	Prednisolone hydrogen suc…	14G29-B07	1
Caelo	Prednisolone hydrogen suc…	15C11B05328275	1
Caelo	Prednisolone hydrogen suc…	15C11-B05-305533	1
Caelo	Prednisolone hydrogen suc…	19081502	1
Fagron	Prednisolone hydrogen suc…	12L14-N04	1
Fagron	Prednisolone hydrogen suc…	14G29-B07-304733	1
Fagron	Prednisolone hydrogen suc…	15c11-B05338297	1
Fagron	Prednisolone hydrogen suc…	15C11-B05-338297	2
Fagron	Prednisolone hydrogen suc…	15C11-B05-344778	5
Phönix	Prednisolone hydrogen suc…	13H24-N04	1

- 236 051 spectra from 1515 *Apo-Ident* customers from a total of 49 247 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Prednisolone hydrogen succinate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prednisolone hydrogen succinate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	160	0	152 802
Type B	0	80	0	202 004
Type C	0	16	0	236 051

The substance/substance group *Prednisolone hydrogen succinate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20956	20956	0.00	82.86
22652	22652	0.00	80.66
22723	22652	3.20	82.30
25644	25644	0.00	83.41

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Prednisone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20002-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Prednisone; Prednisonum

Special notes

When selecting the *Prednisone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Prednisone	6	8	58

Second-stage model

For differentiation of the substance/substance group *Prednisone* the following second-stage model is used:

- Submodel 08

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Prednisone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	69.55	–
⋮	⋮	⋮
Prednisolone acetate	>50	37.12
Ephedrine hydrochloride	>50	137.13

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Prednisone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Prednisone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Prednisone	12232716	21408	60	20120829
Caelo	Prednisone	12232716	21409	60	20120829
Caelo	Prednisone	192455	24895	40	31102019*
Euro OTC	Prednisone	1401042-02	21616	60	1605276
Euro OTC	Prednisone	1604051	22557	40	20160523*
Euro OTC	Prednisone	1604051	22557SI	40	20160523*
Fagron	Prednisone	13C14-B40-289148	21573	60	20131223
Fagron	Prednisone	16J19-B02-328642	23227	40	20161221

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 400 spectra of 8 reference samples from the substance/substance group *Prednisone*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 562 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 769 spectra of 20 reference samples from the substance/substance group *Prednisone*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Prednisone	171665	23341	20
Caelo	Prednisone	17166504	23578	30
Caelo	Prednisone	21003706	25993	40
Caelo	Prednisone	23000981	26974	40
Euro OTC	Prednisone	1702008	23179	40
Fagron	Prednisone	22A14-B08-213641	26133	40
Fagron	Prednisone	23A04-B03-226162	26618	40
Fagron	Prednisone	24A30-B09-237512	27373	40
Caelo	Prednisone	12232716	21408SI†	60
Caelo	Prednisone	12232716	21409SI†	60
Caelo	Prednisone	171665	23341SI	30
Caelo	Prednisone	17166504	23578SI	30
Caelo	Prednisone	192455	24895SI†	40
Caelo	Prednisone	21003706	25993SI	40
Caelo	Prednisone	23000981	26974SI	40
Euro OTC	Prednisone	1702008	23179SI	29
Fagron	Prednisone	16J19-B02-328642	23227SI†	30
Fagron	Prednisone	22A14-B08-213641	26133SI	40
Fagron	Prednisone	23A04-B03-226162	26618SI	40
Fagron	Prednisone	24A30-B09-237512	27373SI	40

- 201 315 spectra from a total of 4034 batches from further 838 substances. These spectra were

recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 104 spectra from 57 *Apo-Ident* customers from 59 batches from the substance/substance group *Prednisone*.
- Among them are spectra of independent samples from 58 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Prednisone	21003706007	1
	Prednisone	21003706008	1
Caelo	Prednisone	10037817	1
Caelo	Prednisone	10037826	1
Caelo	Prednisone	12177604	1
Caelo	Prednisone	12232705	3
Caelo	Prednisone	12232712	1
Caelo	Prednisone	12232713	1
Caelo	Prednisone	12232714	1
Caelo	Prednisone	13262302	1
Caelo	Prednisone	13262304	3
Caelo	Prednisone	15218602	5
Caelo	Prednisone	15218606	5
Caelo	Prednisone	15218607	1
Caelo	Prednisone	16277201	1
Caelo	Prednisone	16277206	1
Caelo	Prednisone	17166501	2
Caelo	Prednisone	17166502	5
Caelo	Prednisone	17166503	1
Caelo	Prednisone	17166504	1
Caelo	Prednisone	17166507	3
Caelo	Prednisone	17166508	2
Caelo	Prednisone	171666508	1
Caelo	Prednisone	18058701	1
Caelo	Prednisone	18108003	1
Caelo	Prednisone	18108004	2
Caelo	Prednisone	19245501	2
Caelo	Prednisone	19245502	1
Caelo	Prednisone	204312107	1
Caelo	Prednisone	21000576001	1
Caelo	Prednisone	21000576002	1
Caelo	Prednisone	21003706002	1
Caelo	Prednisone	21003706003	1
Caelo	Prednisone	21003706005	1
Caelo	Prednisone	21003706007	1
Caelo	Prednisone	2114Q2107	1
Caelo	Prednisone	28021401	1
Caelo	Prednisone	28021403	1
Caelo	Prednisone	5087	1
Caesar & Loretz GmbH...	Prednisone	18108004	1
Caesar & Loretz GmbH	Prednisone	17166508	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Prednisone	18108003	3
Caesar & Loretz GmbH	Prednisone	18108004	1
Caesar & Loretz GmbH	Prednisone	20001277001	1
Caesar & Loretz GmbH	Prednisone	21003706006	1
Euro OTC	Prednisone	1401042-02	1
Euro OTC	Prednisone	150043-03	1
Euro OTC	Prednisone	1501043-01	2
Euro OTC	Prednisone	1501043-02	1
Euro OTC	Prednisone	1501043-03	5
Euro OTC	Prednisone	1604051-01	3
Euro OTC	Prednisone	1604501-01	1
Euro OTC	Prednisone	1702008-01	3
Euro OTC	Prednisone	172008-01	1
Fagron	Prednisone	12E02-N01	1
Fagron	Prednisone	12E02-N10	1
Fagron	Prednisone	13C13-N08	1
Fagron	Prednisone	15218608	1
Fagron	Prednisone	16H04-B04-334368	1
Fagron	Prednisone	20F19-F02-371975	1
Fagron	Prednisone	21021401	1
Gehe	Prednisone	12232714	1
Gehe	Prednisone	12L14-M03	1
Gehe	Prednisone	13C13-N08	1
Gehe	Prednisone	17166508	1
Noweda	Prednisone	17166501	1
Noweda	Prednisone	17166503	1
Noweda	Prednisone	21003060027	1
Phönix	Prednisone	11D08-N05	1
sanacorp	Prednisone	13262302	1
Sanacorp	Prednisone	16277206	1

- 235 963 spectra from 1515 *Apo-Ident* customers from a total of 49 199 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Prednisone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prednisone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	769	0	201 315
Type C	0	102	2	235 963

The substance/substance group *Prednisone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2198 %)
Type C	100.0000 % (> 99.9007 %)	98.0769 % (> 95.1923 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21408	22557	13.72	120.14
21409	22557	10.59	119.25
21573	21616	9.11	120.53
21616	21616	0.00	116.78
22557	22557	0.00	115.59
23227	24895	4.87	114.73
24895	24895	0.00	114.84

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Pregnenolone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20721-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Pregnenolone; Pregnenolonum

Special notes

When selecting the *Pregnenolone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Pregnenolone	11	10	46

Second-stage model

For differentiation of the substance/substance group *Pregnenolone* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Pregnenolone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prasterone	71.51	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Pregnenolone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Pregnenolone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Pregnenolone	1204040-01	20721	40	1404311
Euro OTC	Pregnenolone	1312007-01	21679	60	8985
Euro OTC	Pregnenolone	1602001	22375	45	20160208*
Euro OTC	Pregnenolone	1612019	22979	40	20170131*
Euro OTC	Pregnenolone	1908021	24849	40	20190913*
Euro OTC	Pregnenolone	1908020	24932	40	20191018*
Euro OTC	Pregnenolone	2006014	25325	40	20200803*
Euro OTC	Pregnenolone	2104008	25685	50	20210510*
Fagron	Pregnenolone	15B11-B07-310278	22355	45	9338
Fagron	Pregnenolone	18L27-B02-357840	24704	40	20190220
Fagron	Pregnenolone	22I19-B02	26445	40	20221201*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 480 spectra of 11 reference samples from the substance/substance group *Pregnenolone*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 482 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 460 spectra of 13 reference samples from the substance/substance group *Pregnenolone*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Pregnenolone	1606028	22706	40
Euro OTC	Pregnenolone	1709017	23696	40
Euro OTC	Pregnenolone	1909013	24954	40
Euro OTC	Pregnenolone	2001037	25129	40
Euro OTC	Pregnenolone	2006015	25342	40
Euro OTC	Pregnenolone	2101012	25539	40
Euro OTC	Pregnenolone	2108003	25765	40
Euro OTC	Pregnenolone	2203003	26029	40
Euro OTC	Pregnenolone	2201037	26033	40
Fagron	Pregnenolone	23I28-B11-233503	27057	40
Euro OTC	Pregnenolone	2203003	26029SI	20
Euro OTC	Pregnenolone	2201037	26033SI	20
Fagron	Pregnenolone	23I28-B11-233503	27057SI	20

- 201 624 spectra from a total of 4035 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 231 spectra from 24 *Apo-Ident* customers from 50 batches from the substance/substance group *Pregnenolone*.

- Among them are spectra of independent samples from 46 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Pregnenolone	23D11-B02-226331	1
	Pregnenolone	23I28-B11-233501	1
	Pregnenolone	23I28-B11-233503	1
Audor Pharma	Pregnenolone	A141215/46	1
Audor Pharma	Pregnenolone	AP10L10-M01P	1
Audor Pharma	Pregnenolone	AP1109007-01P	1
Audor Pharma	Pregnenolone	APC07-150801(M)P	3
Audor Pharma	Pregnenolone	APC07-160801(M)P	2
Audor Pharma	Pregnenolone	APc07-180201	1
Audor Pharma	Pregnenolone	APC07-180201	2
Audor Pharma	Pregnenolone	APC07-180201(M)P	3
Audor Pharma	Pregnenolone	APc07-180702(M)-1P	1
Audor Pharma	Pregnenolone	APC07-180702(M)-1P	1
Audor Pharma	Pregnenolone	APC07-180702(M)-2P	1
bitte ergänzen	Pregnenolone		1
Euro OTC	Pregnenolone	1312007-01	1
Euro OTC	Pregnenolone	1402025-01	1
Euro OTC	Pregnenolone	1506002-01	10
Euro OTC	Pregnenolone	1602001-01	22
Euro OTC	Pregnenolone	1606028-01	29
Euro OTC	Pregnenolone	1612019-01	51
Euro OTC	Pregnenolone	1908021-01	2
Euro OTC	Pregnenolone	1908021-02	1
Euro OTC	Pregnenolone	2001037-01	24
Euro OTC	Pregnenolone	2001037-02	3
Euro OTC	Pregnenolone	2006015-01	5
Euro OTC	Pregnenolone	2006015-02	36
Euro OTC	Pregnenolone	2101012-01	2
Euro OTC	Pregnenolone	2108003-01	1
Euro OTC	Pregnenolone	2203003-01	2
Fagron	Pregnenolone	14B18-B04-291917	1
Fagron	Pregnenolone	16L29-B02331611	1
Fagron	Pregnenolone	19E01-B01-364473	1
Fagron	Pregnenolone	19J25-F02	1
Fagron	Pregnenolone	19J25-F02-367245	1
Fagron	Pregnenolone	19L09-F01-372068	1
Fagron	Pregnenolone	20104-F04-378102	1
Fagron	Pregnenolone	20I04-F04-374073	1
Fagron	Pregnenolone	23G20-B02-233060	1
Fagron	Pregnenolone	23I28-B11-233499	1
Fagron	Pregnenolone	F01-3720608	1
Fagron	Pregnenolone	F02-3672405	1
Fagron	Pregnenolone	F04-3784905	1
gehe	Pregnenolone	Apc07160801	1
Haihang Industry	Pregnenolone	20140329	1
Koisser Pharma	Pregnenolone	ZH-131001	1
Koisser	Pregnenolone	ZH-130802	1
KS Pharma	Pregnenolone	ZH-111119	1
NWM CHina	Pregnenolone	PR150329	1
NWM Shandong Northwe...	Pregnenolone	PRN151219	1

- 235 836 spectra from 1515 *Apo-Ident* customers from a total of 49 209 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Pregnenolone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pregnenolone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	480	0	152 482
Type B	0	460	0	201 624
Type C	0	226	5	235 836

The substance/substance group *Pregnenolone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.6957 %)
Type C	100.0000 % (> 99.9007 %)	97.8355 % (> 96.5368 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20721	20721	0.00	92.66
21679	21679	0.00	92.42
22355	22355	0.00	97.80
22375	22375	0.00	92.67
22979	22979	0.00	93.73
24704	26445	7.28	96.69
24849	24849	0.00	93.05
24932	24932	0.00	96.87
25325	25325	0.00	96.73
25685	25685	0.00	98.15
26445	26445	0.00	95.59

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Prilocaine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10005414-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Prilocaine; Prilocainum

Special notes

When selecting the *Prilocaine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Prilocaine	2	1	0

Second-stage model

For differentiation of the substance/substance group *Prilocaine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Prilocaine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	121.97	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Prilocaine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Prilocaine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Prilocaine	2208012	26336	40	20221018*
Euro OTC	Prilocaine	2310022	27370	40	20240826*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Prilocaine*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 882 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 3 reference samples from the substance/substance group *Prilocaine*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Prilocaine	1909017-01	25782	50
Euro OTC	Prilocaine	2208012	26336SI†	20
Euro OTC	Prilocaine	2310022	27370SI†	20

- 201 994 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Prilocaine*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Prilocaine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

relevant spectra of the various substances were compared with *Prilocaine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	80	0	152 882
Type B	0	87	3	201 994
Type C	0	0	0	236 067

The substance/substance group *Prilocaine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9912 %)	96.6667 % (> 93.3333 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26336	26336	0.00	197.90
27370	27370	0.00	200.10

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Prilocaine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21048-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Prilocaine hydrochloride; Prilocaini hydrochloridum

Special notes

When selecting the *Prilocaine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Prilocaine hydrochloride	4	3	20

Second-stage model

For differentiation of the substance/substance group *Prilocaine hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Prilocaine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Amphetamine sulfate	79.14	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Prilocaine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Prilocaine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Prilocaine hydrochloride	15230305	21926	60	20150723
Fagron	Prilocaine hydrochloride	13I02-N03	21048	40	1403257
Fagron	Prilocaine hydrochloride	13I02-N03	21050	40	20130918
Fagron	Prilocaine hydrochloride	14H13-B03-297591	21800	60	AR-15-FG-016323-01
Fagron	Prilocaine hydrochloride	23A13-B01-225390	26612	40	20230208

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 5 reference samples from the substance/substance group *Prilocaine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 722 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 5 reference samples from the substance/substance group *Prilocaine hydrochloride*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Prilocaine hydrochloride	15390101	23250	40
Fagron	Prilocaine hydrochloride	20B25-F04-369313	25484	40
Fagron	Prilocaine hydrochloride	24A16-B11-234645	27187	40
Fagron	Prilocaine hydrochloride	23A13-B01-225390	26612SI†	20
Fagron	Prilocaine hydrochloride	24A16-B11-234645	27187SI	20

- 201 924 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 35 spectra from 22 *Apo-Ident* customers from 23 batches from the substance/substance group *Prilocaine hydrochloride*.

- Among them are spectra of independent samples from 19 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Prilocaine hydrochloride	21G10-B21-213674	1
Caelo	Prilocaine hydrochloride	14A03-B34-290281	1
Caelo	Prilocaine hydrochloride	15230304	1
Caelo	Prilocaine hydrochloride	15230305	1
Caelo	Prilocaine hydrochloride	15390101	1
Fagron	Prilocaine hydrochloride		1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Prilocaine hydrochloride	13I032-N03	1
Fagron	Prilocaine hydrochloride	14H13-B03-297591	1
Fagron	Prilocaine hydrochloride	14H13-B03-297593	1
Fagron	Prilocaine hydrochloride	15E15-B04-307730	1
Fagron	Prilocaine hydrochloride	15L21-B02_332956	1
Fagron	Prilocaine hydrochloride	15L21-B02-319234	1
Fagron	Prilocaine hydrochloride	15L21-B02325756	1
Fagron	Prilocaine hydrochloride	15L21-B02332956	1
Fagron	Prilocaine hydrochloride	15L21-B02-332956	2
Fagron	Prilocaine hydrochloride	17H02-B05-340539	3
Fagron	Prilocaine hydrochloride	17H02-B05-348769	5
Fagron	Prilocaine hydrochloride	17Ho2Bo5348769	1
Fagron	Prilocaine hydrochloride	18B22-B04-356468	1
Fagron	Prilocaine hydrochloride	21F07-B14	1
Fagron	Prilocaine hydrochloride	21G10-B21-213674	3
Fagron	Prilocaine hydrochloride	F04-3766906	3
Fargon	Prilocaine hydrochloride	17HO2-B05	1
GEHE 02.05.2013	Prilocaine hydrochloride		1

- 236 032 spectra from 1515 *Apo-Ident* customers from a total of 49 236 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Prilocaine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Prilocaine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	240	0	152 722
Type B	0	160	0	201 924
Type C	0	35	0	236 032

The substance/substance group *Prilocaine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 82.8571 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21048	21048	0.00	101.52
21050	21048	3.52	102.24
21800	21800	0.00	104.65
21926	21800	4.59	101.43
26612	21048	11.17	104.73

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Procaine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20042-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Procaine hydrochloride; Procaini hydrochloridum

Special notes

When selecting the *Procaine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Procaine hydrochloride	8	7	88

Second-stage model

For differentiation of the substance/substance group *Procaine hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Procaine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	148.91	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Procaine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Procaine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Procaine hydrochloride	13109906	21785	60	AR-15-FG-008935-01
Caelo	Procaine hydrochloride	15006906	22247	60	20150209
Caelo	Procaine hydrochloride	19000709003	25436	40	20200120
Caelo	Procaine hydrochloride	23000279004	26742	40	20230306
Caelo	Procaine hydrochloride	23000279004	26742SI	20	20230306
Euro OTC	Procaine hydrochloride	1601014	22306	60	20160203*
Euro OTC	Procaine hydrochloride	2210004	26442	40	20221116*
Fagron	Procaine hydrochloride	13F12-B40-301798	22260	60	20141210
Fagron	Procaine hydrochloride	15J27-B10-322937	23379	40	20151113

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 420 spectra of 9 reference samples from the substance/substance group *Procaine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 542 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 310 spectra of 9 reference samples from the substance/substance group *Procaine hydrochloride*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Procaine hydrochloride	161378	22624	40
Caelo	Procaine hydrochloride	171675	23634	40
Caelo	Procaine hydrochloride	182764	24393	40
Caelo	Procaine hydrochloride	190440	24526	40
Caelo	Procaine hydrochloride	21003774005	26307	40
Caelo	Procaine hydrochloride	24001422	27309	30
Fagron	Procaine hydrochloride	22K02-B01-226161	26552	40
Caelo	Procaine hydrochloride	21003774005	26307SI	20
Fagron	Procaine hydrochloride	22K02-B01-226161	26552SI	20

- 201 774 spectra from a total of 4038 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 208 spectra from 133 *Apo-Ident* customers from 92 batches from the substance/substance group *Procaine hydrochloride*.

- Among them are spectra of independent samples from 88 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Procaine hydrochloride	21003774005	1
	Procaine hydrochloride	22002755005	1
	Procaine hydrochloride	23000279003	1
	Procaine hydrochloride	23000279004	2
	Procaine hydrochloride	23000279007	1
	Procaine hydrochloride	23000279008	1
	Procaine hydrochloride	3000279004	1
Alliance Health 09.0...	Procaine hydrochloride	1104012-05	1
Anzag	Procaine hydrochloride	60998058	1
Caelo	Procaine hydrochloride	10159721	1
Caelo	Procaine hydrochloride	10159723	1
Caelo	Procaine hydrochloride	10159729	1
Caelo	Procaine hydrochloride	11370203	1
Caelo	Procaine hydrochloride	11370204	1
Caelo	Procaine hydrochloride	11370206	1
Caelo	Procaine hydrochloride	11370215	1
Caelo	Procaine hydrochloride	11370216	2
Caelo	Procaine hydrochloride	11370219	1
Caelo	Procaine hydrochloride	12177801	5
Caelo	Procaine hydrochloride	13/09-N08	1
Caelo	Procaine hydrochloride	13109905	1
Caelo	Procaine hydrochloride	13109906	1
Caelo	Procaine hydrochloride	13109908	2
Caelo	Procaine hydrochloride	13109915	1
Caelo	Procaine hydrochloride	13109916	2
Caelo	Procaine hydrochloride	131099903	1
Caelo	Procaine hydrochloride	13130-N06	1
Caelo	Procaine hydrochloride	13F12-B40-302510	1
Caelo	Procaine hydrochloride	14164408	1
Caelo	Procaine hydrochloride	14164409	1
Caelo	Procaine hydrochloride	14164413	1
Caelo	Procaine hydrochloride	15006902	1
Caelo	Procaine hydrochloride	15006906	3
Caelo	Procaine hydrochloride	15006909	1
Caelo	Procaine hydrochloride	15006912	4
Caelo	Procaine hydrochloride	15006913	1
Caelo	Procaine hydrochloride	1601014-02	1
Caelo	Procaine hydrochloride	16137812	5
Caelo	Procaine hydrochloride	16173906	2
Caelo	Procaine hydrochloride	17167504	1
Caelo	Procaine hydrochloride	17167505	1
Caelo	Procaine hydrochloride	17167506	2
Caelo	Procaine hydrochloride	17343306	1
Caelo	Procaine hydrochloride	17343311	1
Caelo	Procaine hydrochloride	18041806	1
Caelo	Procaine hydrochloride	18276407	4
Caelo	Procaine hydrochloride	19000709001	1
Caelo	Procaine hydrochloride	19000709003	9
Caelo	Procaine hydrochloride	19044008	2
Caelo	Procaine hydrochloride	192848001	1
Caelo	Procaine hydrochloride	192848002	7
Caelo	Procaine hydrochloride	192848005	1
Caelo	Procaine hydrochloride	20001278003	3
Caelo	Procaine hydrochloride	20001278004	2
Caelo	Procaine hydrochloride	20001278005	1
Caelo	Procaine hydrochloride	20004565003	3
Caelo	Procaine hydrochloride	20004565004	1
Caelo	Procaine hydrochloride	21003774002	6
Caelo	Procaine hydrochloride	22002755005	1
Caelo	Procaine hydrochloride	60998127	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Procaine hydrochloride	7011506	1
Caesar & Loretz GmbH...	Procaine hydrochloride	23000279004	1
Caesar & Loretz GmbH	Procaine hydrochloride	14164413	1
Caesar & Loretz GmbH	Procaine hydrochloride	17343306	1
Caesar & Loretz GmbH	Procaine hydrochloride	18276407	1
Caesar & Loretz GmbH	Procaine hydrochloride	19000709003	1
Caesar & Loretz GmbH	Procaine hydrochloride	19044008	1
CAESAR & LORETZ GMBH	Procaine hydrochloride	192848001	2
Caesar & Loretz GmbH	Procaine hydrochloride	192848005	1
Caesar & Loretz GmbH	Procaine hydrochloride	20001278003	1
Caesar & Loretz GmbH	Procaine hydrochloride	20004565003	1
Caesar & Loretz GmbH	Procaine hydrochloride	21003774002	1
Caesar & Loretz GmbH	Procaine hydrochloride	21003774005	3
Caesar & Loretz GmbH	Procaine hydrochloride	21003775002	1
China Medica	Procaine hydrochloride	13109911	1
Chongging Southwest No.2	Procaine hydrochloride	20001278004	1
Euro OTC	Procaine hydrochloride	1003001-01	1
Euro OTC	Procaine hydrochloride	1003001-02	1
Euro OTC	Procaine hydrochloride	1104012-01	1
Euro OTC	Procaine hydrochloride	1104012-03	3
Euro OTC	Procaine hydrochloride	1104012-04	3
Euro OTC	Procaine hydrochloride	1104012-05	4
Euro OTC	Procaine hydrochloride	1104012-3	1
Euro OTC	Procaine hydrochloride	1405027-01	4
Euro OTC	Procaine hydrochloride	1405027-02	1
Euro OTC	Procaine hydrochloride	16001014-02	1
Euro OTC	Procaine hydrochloride	1601014-01	9
Euro OTC	Procaine hydrochloride	1601014-02	22
Euro OTC	Procaine hydrochloride	1601014-02	1
Euro OTC	Procaine hydrochloride	16014014-02	1
Euro OTC	Procaine hydrochloride	200644	1
Euro OTC	Procaine hydrochloride	5127	1
Fagron	Procaine hydrochloride	10H11-N25	1
Fagron	Procaine hydrochloride	12I10-N07	1
Fagron	Procaine hydrochloride	13/30-N06	1
Fagron	Procaine hydrochloride	13F12-B40	1
Fagron	Procaine hydrochloride	13I09-N08	1
Fagron	Procaine hydrochloride	15006906	1
Fagron	Procaine hydrochloride	1651212	1
Fagron	Procaine hydrochloride	193768	1
Fagron	Procaine hydrochloride	20A30-B15-197566	1
Gatt-Koller / Phoenix	Procaine hydrochloride	4428/10122714	2
Gehe	Procaine hydrochloride	19044008	1
Guzugzhou Tengyue Ch...	Procaine hydrochloride	20201033	2
Herstellung	Procaine hydrochloride	12177801	1
Koisser	Procaine hydrochloride	11370218	1
Nachprüfung	Procaine hydrochloride	2082019-5	1
Noweda	Procaine hydrochloride	1309N08	1
Noweda	Procaine hydrochloride	1601014-02	1
Noweda	Procaine hydrochloride	22002755005	1
Noweda	Procaine hydrochloride	23000279004	1
Phönix 08.01.2014	Procaine hydrochloride	1104012-03	1
Phönix Gotha	Procaine hydrochloride	190311	1
Sanacorp	Procaine hydrochloride	20004565003	1
siehe WE-Prüfprotokoll	Procaine hydrochloride	39/12	1
VEB Jenapharmn	Procaine hydrochloride	1011989	1

- 235 859 spectra from 1515 *Apo-Ident* customers from a total of 49 166 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are docu-

mented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Procaine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Procaine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	310	0	201 774
Type C	0	208	0	235 859

The substance/substance group *Procaine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.0645 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 97.1154 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21785	21785	0.00	197.01
22247	22306	6.74	199.31
22260	21785	6.88	198.14
22306	22306	0.00	197.16
23379	22306	3.21	197.44
25436	26442	13.77	202.75
26442	26442	0.00	201.13
26742	26442	9.42	203.92

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Progesterone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20024-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Progesterone; Progesteronum

Special notes

When selecting the *Progesterone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Progesterone	14	79	558

Second-stage model

For differentiation of the substance/substance group *Progesterone* the following second-stage model is used:

- Submodel 05

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Progesterone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Spironolactone	61.73	58.50
⋮	⋮	⋮
Testosterone propionate	>50	54.15
Povidone	>50	106.84
Fusidic acid	>50	110.88
Povidone iodine	>50	123.57
Ubidecarenone	>50	127.08

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Progesterone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Progesterone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Progesterone	15319601	22831	40	20151014
Caelo	Progesterone	17060903	23249	40	20170315
Caelo	Progesterone	20002672	25658	50	20200914*
Caelo	Progesterone	20002672	25658SI	50	20200914*
Euro OTC	Progesterone	1111053-01	20718	30	20120119
Euro OTC	Progesterone	1506033	21868	60	0000010482
Euro OTC	Progesterone	1506033	21868SI	30	0000010482
Euro OTC	Progesterone	1506034	21870	60	0000010483
Euro OTC	Progesterone	1509008	21907	60	20150914*
Euro OTC	Progesterone	1511008	22226	60	20151119*
Euro OTC	Progesterone	1601009	22301	45	20160128*
Euro OTC	Progesterone	1601009	22301SI	45	20160128*
Euro OTC	Progesterone	1601001	22303	45	20160128*
Euro OTC	Progesterone	1603004	22525	40	20160406*
Euro OTC	Progesterone	2006018	25273	40	20200716*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Progesterone	2006018	25273SI	31	20200716*
Euro OTC	Progesterone	2103019	25684	50	20210427*
Euro OTC	Progesterone	2103019	25684SI	50	20210427*
Fagron	Progesterone	16A20-B02-319103	22830	40	20160209
Fagron	Progesterone	16A20-B02-319103	22830SI	40	20160209

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 906 spectra of 20 reference samples from the substance/substance group *Progesterone*. These samples are listed above in the *calibration samples* section. The reference samples come from 14 different batches.

- 152 056 spectra from a total of 2828 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 6386 spectra of 168 reference samples from the substance/substance group *Progesterone*.

- Among them are spectra of independent samples from 79 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Progesterone	170609	23329	40
Caelo	Progesterone	172778	23838	40
Caelo	Progesterone	191287	24750	40
Caelo	Progesterone	21002413	25792	40
Caelo	Progesterone	22001580	26252	40
Caelo	Progesterone	22001577	26256	40
Caelo	Progesterone	22003208	26485	40
Caelo	Progesterone	23003401	27104	40
Euro OTC	Progesterone	1603012	22529	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Progesterone	1605013	22556	40
Euro OTC	Progesterone	1606033	22704	40
Euro OTC	Progesterone	1605032	22705	40
Euro OTC	Progesterone	1609016	22788	40
Euro OTC	Progesterone	1609001	22819	40
Euro OTC	Progesterone	1701038	23138	40
Euro OTC	Progesterone	1702026	23148	40
Euro OTC	Progesterone	1707012	23536	40
Euro OTC	Progesterone	1705028	23541	40
Euro OTC	Progesterone	1709012	23732	40
Euro OTC	Progesterone	1801036	23947	40
Euro OTC	Progesterone	1802030	24067	40
Euro OTC	Progesterone	1806020	24138	40
Euro OTC	Progesterone	1809018	24328	40
Euro OTC	Progesterone	1809017	24334	40
Euro OTC	Progesterone	1603012-01	24335	40
Euro OTC	Progesterone	1811033	24345	40
Euro OTC	Progesterone	1901021	24447	40
Euro OTC	Progesterone	1901022	24455	40
Euro OTC	Progesterone	1904033	24606	40
Euro OTC	Progesterone	1905023	24765	40
Euro OTC	Progesterone	1905022	24790	40
Euro OTC	Progesterone	1908002	24834	40
Euro OTC	Progesterone	1908003	24863	40
Euro OTC	Progesterone	1911006	24962	40
Euro OTC	Progesterone	1911007	24970	40
Euro OTC	Progesterone	2001036	25077	40
Euro OTC	Progesterone	2003037	25110	40
Euro OTC	Progesterone	2003042	25111	40
Euro OTC	Progesterone	2003036	25112	40
Euro OTC	Progesterone	2005019	25255	40
Euro OTC	Progesterone	2005018	25256	40
Euro OTC	Progesterone	2007029	25262	40
Euro OTC	Progesterone	2006017	25263	40
Euro OTC	Progesterone	2007028	25276	40
Euro OTC	Progesterone	2010005	25474	40
Euro OTC	Progesterone	2103020	25683	50
Euro OTC	Progesterone	2108010	25819	50
Euro OTC	Progesterone	2108011	25831	50
Euro OTC	Progesterone	2111009	25917	40
Euro OTC	Progesterone	2111008	25921	40
Euro OTC	Progesterone	2203007	26032	40
Euro OTC	Progesterone	2203006	26034	40
Euro OTC	Progesterone	2207002	26214	40
Euro OTC	Progesterone	2210017	26425	40
Euro OTC	Progesterone	2210016	26443	40
Euro OTC	Progesterone	2301049	26577	30
Euro OTC	Progesterone	2307007	26760	40
Euro OTC	Progesterone	2307006	26761	40
Euro OTC	Progesterone	2308001	26886	30
Euro OTC	Progesterone	2308002	26887	30
Euro OTC	Progesterone	2309026	26937	40
Euro OTC	Progesterone	2311009	27013	40
Euro OTC	Progesterone	2311010	27014	40
Euro OTC	Progesterone	2401013	27088	40
Euro OTC	Progesterone	2401014	27089	40
Euro OTC	Progesterone	2402023	27143	40
Euro OTC	Progesterone	2404001	27203	40
Euro OTC	Progesterone	2404005	27204	40
Euro OTC	Progesterone	2405006	27205	40

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Progesterone	2405005	27208	40
Euro OTC	Progesterone	2406015	27284	40
Euro OTC	Progesterone	2406014	27285	40
Euro OTC	Progesterone	2407018	27354	40
Euro OTC	Progesterone	2407019	27355	30
Euro OTC	Progesterone	2409003	27398	40
Euro OTC	Progesterone	2410011	27461	40
Euro OTC	Progesterone	2410010	27462	40
Fagron	Progesterone	19H20-F02-364866	25046	40
Fagron	Progesterone	22H12-B01-222409	26407	40
Caelo	Progesterone	15319601	22831SI†	40
Caelo	Progesterone	17060903	23249SI†	20
Caelo	Progesterone	170609	23329SI	20
Caelo	Progesterone	172778	23838SI	30
Caelo	Progesterone	170609	23844	40
Caelo	Progesterone	170609	23844SI	23
Caelo	Progesterone	191287	24750SI	40
Caelo	Progesterone	21002413	25792SI	40
Caelo	Progesterone	22001580	26252SI	40
Caelo	Progesterone	22001577	26256SI	40
Caelo	Progesterone	22003208	26485SI	35
Caelo	Progesterone	23003401	27104SI	20
Euro OTC	Progesterone	1506033	21868SI†	20
Euro OTC	Progesterone	1506034	21870SI†	59
Euro OTC	Progesterone	1509008	21907SI†	53
Euro OTC	Progesterone	1511008	22226SI†	27
Euro OTC	Progesterone	1601001	22303SI†	44
Euro OTC	Progesterone	1603004	22525SI†	31
Euro OTC	Progesterone	1603012	22529SI	29
Euro OTC	Progesterone	1605013	22556SI	30
Euro OTC	Progesterone	1606033	22704SI	30
Euro OTC	Progesterone	1605032	22705SI	38
Euro OTC	Progesterone	1609016	22788SI	30
Euro OTC	Progesterone	1609001	22819SI	30
Euro OTC	Progesterone	1701038	23138SI	20
Euro OTC	Progesterone	1702026	23148SI	20
Euro OTC	Progesterone	1707012	23536SI	28
Euro OTC	Progesterone	1705028	23541SI	25
Euro OTC	Progesterone	1709012	23732SI	40
Euro OTC	Progesterone	1801036	23947SI	20
Euro OTC	Progesterone	1802030	24067SI	32
Euro OTC	Progesterone	1806020	24138SI	35
Euro OTC	Progesterone	1809018	24328SI	30
Euro OTC	Progesterone	1809017	24334SI	40
Euro OTC	Progesterone	1603012-01	24335SI	20
Euro OTC	Progesterone	1811033	24345SI	30
Euro OTC	Progesterone	1901021	24447SI	40
Euro OTC	Progesterone	1901022	24455SI	40
Euro OTC	Progesterone	1904033	24606SI	39
Euro OTC	Progesterone	1905023	24765SI	40
Euro OTC	Progesterone	1905022	24790SI	40
Euro OTC	Progesterone	1908002	24834SI	40
Euro OTC	Progesterone	1908003	24863SI	40
Euro OTC	Progesterone	1911006	24962SI	40
Euro OTC	Progesterone	1911007	24970SI	40
Euro OTC	Progesterone	2001036	25077SI	40
Euro OTC	Progesterone	2003037	25110SI	40
Euro OTC	Progesterone	2003042	25111SI	40
Euro OTC	Progesterone	2003036	25112SI	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Progesterone	2005019	25255SI	30
Euro OTC	Progesterone	2005018	25256SI	40
Euro OTC	Progesterone	2007029	25262SI	39
Euro OTC	Progesterone	2006017	25263SI	40
Euro OTC	Progesterone	2007028	25276SI	40
Euro OTC	Progesterone	2010005	25474SI	40
Euro OTC	Progesterone	2103020	25683SI	50
Euro OTC	Progesterone	2108010	25819SI	50
Euro OTC	Progesterone	2108011	25831SI	50
Euro OTC	Progesterone	2111009	25917SI	40
Euro OTC	Progesterone	2111008	25921SI	40
Euro OTC	Progesterone	2203007	26032SI	40
Euro OTC	Progesterone	2203006	26034SI	40
Euro OTC	Progesterone	2207002	26214SI	40
Euro OTC	Progesterone	2210017	26425SI	40
Euro OTC	Progesterone	2210016	26443SI	40
Euro OTC	Progesterone	2301049	26577SI	40
Euro OTC	Progesterone	2307007	26760SI	40
Euro OTC	Progesterone	2307006	26761SI	40
Euro OTC	Progesterone	2308001	26886SI	31
Euro OTC	Progesterone	2308002	26887SI	31
Euro OTC	Progesterone	2309026	26937SI	40
Euro OTC	Progesterone	2311009	27013SI	35
Euro OTC	Progesterone	2311010	27014SI	40
Euro OTC	Progesterone	2401013	27088SI	35
Euro OTC	Progesterone	2401014	27089SI	40
Euro OTC	Progesterone	2402023	27143SI	40
Euro OTC	Progesterone	2404001	27203SI	38
Euro OTC	Progesterone	2404005	27204SI	35
Euro OTC	Progesterone	2405006	27205SI	39
Euro OTC	Progesterone	2405005	27208SI	40
Euro OTC	Progesterone	2406015	27284SI	40
Euro OTC	Progesterone	2406014	27285SI	36
Euro OTC	Progesterone	2407018	27354SI	40
Euro OTC	Progesterone	2407019	27355SI	39
Euro OTC	Progesterone	2409003	27398SI	40
Euro OTC	Progesterone	2410011	27461SI	30
Euro OTC	Progesterone	2410010	27462SI	40
Fagron	Progesterone	19H20-F02-364866	25046SI	40
Fagron	Progesterone	22H12-B01-222409	26407SI	40

- 195 698 spectra from a total of 3958 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3247 spectra from 474 *Apo-Ident* customers from 582 batches from the substance/substance group *Progesterone*.

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- Among them are spectra of independent samples from 557 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Progesterone	1401002-01	2
	Progesterone	14253906	1
	Progesterone	20F-F12-372268	1
	Progesterone	21001388011	2
	Progesterone	21001388017	1
	Progesterone	21001388020	1
	Progesterone	2108010-01	1
	Progesterone	22001580002	1
	Progesterone	22001580003	1
	Progesterone	22003208002	1
	Progesterone	22041400M	1
	Progesterone	2207002-01	2
	Progesterone	2210016-01	1
	Progesterone	22A31-F02-381709	1
	Progesterone	22A31-F02-381712	1
	Progesterone	22H12-B01-222409	3
	Progesterone	22H12-B01-222410	1
	Progesterone	22K17-B10-224492	1
	Progesterone	23002143002	1
	Progesterone	23002143003	5
	Progesterone	2301049-01	3
	Progesterone	2307006-01	1
	Progesterone	2307007-01	1
	Progesterone	2308001-01	1
	Progesterone	2309026-01	2
	Progesterone	2309026-02	2
	Progesterone	2311009-01	1
	Progesterone	23B08B03227299	1
	Progesterone	23B08-B03-227300	1
	Progesterone	23H07-B03-230995	1
	Progesterone	23H07-B04-230996	3
	Progesterone	23H07-B04-230997	4
	Progesterone	2401013-01	2
	Progesterone	2401013-02	1
	Progesterone	2404005-01	3
	Progesterone	2405005-01	1
	Progesterone	2406014-01	1
	Progesterone	C01-230408	1
	Progesterone	EU-HTT230308M	1
A.H. 03.06.13 ek: 6,50EUR	Progesterone	1304014-01	1
AHD	Progesterone	13I11-N11	1
Alliance Healthcare	Progesterone	1206024-02	1
Alliance	Progesterone	15i11-b05-315224	1
Alliance	Progesterone	15I11-B05-315224	2
Anzag 07.04.2016	Progesterone	APC01-150708P	1
ANZAG	Progesterone	12195907	2
Anzag	Progesterone	13K28-B01-293478	1
Anzag	Progesterone	14k11-b04-300921	1
Anzag	Progesterone	15C31-B06-312963	3
Anzag	Progesterone	2515A-03235	1
Audor Pharma	Progesterone	APC01-120613P	1
Audor Pharma	Progesterone	APC01-120708P	3
Audor Pharma	Progesterone	APC01-141212P	1
Audor Pharma	Progesterone	APC01-150311P	1
Audor Pharma	Progesterone	APC01-150708P	5
Audor Pharma	Progesterone	APC01-151114P	9
Audor Pharma	Progesterone	APC01-160201	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Audor Pharma	Progesterone	APC01-160201P	8
Audor Pharma	Progesterone	APC01-170828P	1
Audor Pharma	Progesterone	APC01-171101P	31
Audor Pharma	Progesterone	APC01-180128P	1
Audor Pharma	Progesterone	APC01-180610P	12
Audor Pharma	Progesterone	APC01-181003P	15
Audor Pharma	Progesterone	APC01-181003P	1
Audor Pharma	Progesterone	APOC01-1700828P	2
Audor Pharma	Progesterone	C01-120708P	1
Audor Pharma	Progesterone	C01-180128	10
cae	Progesterone	20004530001	1
Caelo	Progesterone	11177207	1
Caelo	Progesterone	11177219	3
Caelo	Progesterone	11177221	2
Caelo	Progesterone	117348404	1
Caelo	Progesterone	12195828	1
Caelo	Progesterone	12195902	1
Caelo	Progesterone	12195905	3
Caelo	Progesterone	12195906	4
Caelo	Progesterone	12195907	4
Caelo	Progesterone	12195912	3
Caelo	Progesterone	12195913	3
Caelo	Progesterone	12195914	3
Caelo	Progesterone	12195920	8
Caelo	Progesterone	12195924	10
Caelo	Progesterone	12195926	19
Caelo	Progesterone	12195928	7
Caelo	Progesterone	12A19-N04	2
Caelo	Progesterone	130404002	2
Caelo	Progesterone	13155902	10
Caelo	Progesterone	13155920	1
Caelo	Progesterone	13155921	2
Caelo	Progesterone	13155927	4
Caelo	Progesterone	13155928	3
Caelo	Progesterone	13155929	1
Caelo	Progesterone	13G11-N02	1
Caelo	Progesterone	13HI01-N03	1
Caelo	Progesterone	140100201	1
Caelo	Progesterone	14253911	6
Caelo	Progesterone	14253915	2
Caelo	Progesterone	14253929	1
Caelo	Progesterone	14253930	1
Caelo	Progesterone	14H13-B05-3002016	1
Caelo	Progesterone	14K11-B04-300920	2
Caelo	Progesterone	1511-B05-313598	1
Caelo	Progesterone	15124902	1
Caelo	Progesterone	15124910	4
Caelo	Progesterone	15124919	2
Caelo	Progesterone	15319601	7
Caelo	Progesterone	15319602	1
Caelo	Progesterone	15319603	42
Caelo	Progesterone	15319604	1
Caelo	Progesterone	15319607	3
Caelo	Progesterone	15319608	7
Caelo	Progesterone	15319618	4
Caelo	Progesterone	15319619	1
Caelo	Progesterone	15319620	1
Caelo	Progesterone	15C31-808	1
Caelo	Progesterone	15C31-B06-308796	2
Caelo	Progesterone	15I11-B05	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Progesterone	15I11-B05-314184	2
Caelo	Progesterone	160100902	1
Caelo	Progesterone	16015B14-315279	1
Caelo	Progesterone	1605013-02	1
Caelo	Progesterone	16103601	2
Caelo	Progesterone	16103602	4
Caelo	Progesterone	16103603	11
Caelo	Progesterone	16103604	1
Caelo	Progesterone	16103605	3
Caelo	Progesterone	16103606	12
Caelo	Progesterone	16103607	1
Caelo	Progesterone	16103609	30
Caelo	Progesterone	16103610	4
Caelo	Progesterone	16103613	20
Caelo	Progesterone	161036303	9
Caelo	Progesterone	16203605	1
Caelo	Progesterone	16A20-B02-319103	1
Caelo	Progesterone	16D13-B04	1
Caelo	Progesterone	16J05-B04-328263	1
Caelo	Progesterone	16L29-B03-330995	1
Caelo	Progesterone	17/21-B03-343284	1
Caelo	Progesterone	17060901	41
Caelo	Progesterone	17060903	6
Caelo	Progesterone	17060904	6
Caelo	Progesterone	17060905	2
Caelo	Progesterone	17060907	10
Caelo	Progesterone	17060909	13
Caelo	Progesterone	17060910	3
Caelo	Progesterone	17060911	2
Caelo	Progesterone	1706093	1
Caelo	Progesterone	17149903	1
Caelo	Progesterone	17149904	9
Caelo	Progesterone	17149905	1
Caelo	Progesterone	17149906	10
Caelo	Progesterone	17149907	1
Caelo	Progesterone	1719907	10
Caelo	Progesterone	1721bo3342134	1
Caelo	Progesterone	17277801	22
Caelo	Progesterone	1734801	1
Caelo	Progesterone	1734804	2
Caelo	Progesterone	17348401	2
Caelo	Progesterone	17348402	6
Caelo	Progesterone	17348403	10
Caelo	Progesterone	17348404	13
Caelo	Progesterone	17348405	3
Caelo	Progesterone	17348407	7
Caelo	Progesterone	17348409	5
Caelo	Progesterone	1760911	1
Caelo	Progesterone	17C15-B03-333671	1
Caelo	Progesterone	17I21-B03-342136	1
Caelo	Progesterone	1801036-01	16
Caelo	Progesterone	18098801	25
Caelo	Progesterone	182632802	1
Caelo	Progesterone	1826380	1
Caelo	Progesterone	182638004	5
Caelo	Progesterone	182638005	5
Caelo	Progesterone	182638009	1
Caelo	Progesterone	18263801	3
Caelo	Progesterone	182638010	16
Caelo	Progesterone	18263802	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Progesterone	18263804	15
Caelo	Progesterone	18263807	4
Caelo	Progesterone	18263809	9
Caelo	Progesterone	18263811	1
Caelo	Progesterone	18B06-B10	3
Caelo	Progesterone	18B06-B10-346702	1
Caelo	Progesterone	18F22-B04-351435	1
Caelo	Progesterone	18f22-B04-354899	1
Caelo	Progesterone	18F22-B04-355395	1
Caelo	Progesterone	19000591002	13
Caelo	Progesterone	19000591005	7
Caelo	Progesterone	19051502	1
Caelo	Progesterone	19128702	1
Caelo	Progesterone	19128705	2
Caelo	Progesterone	19A25-B01-360449	3
Caelo	Progesterone	19A25-B01-360450	1
Caelo	Progesterone	20004178001	1
Caelo	Progesterone	20004179001	5
Caelo	Progesterone	20004530002	6
Caelo	Progesterone	20004530003	2
Caelo	Progesterone	200303701	1
Caelo	Progesterone	2005019-01	1
Caelo	Progesterone	2006500002	1
Caelo	Progesterone	21001388	1
Caelo	Progesterone	21001388001	1
Caelo	Progesterone	21001388003	6
Caelo	Progesterone	21001388007	2
Caelo	Progesterone	21001388008	1
Caelo	Progesterone	21001388010	2
Caelo	Progesterone	21001388020	3
Caelo	Progesterone	2100138804	1
Caelo	Progesterone	21002413001	1
Caelo	Progesterone	258/61	1
Caelo	Progesterone	27121303	1
Caelo	Progesterone	4814A-03235	1
Caelo	Progesterone	4817Q-03235	1
Caelo	Progesterone	7101401	1
Caelo	Progesterone	9031705	1
Caelo	Progesterone	9195408	1
Caelo	Progesterone	9195429	1
Caelo	Progesterone	B03333671	1
Caelo	Progesterone	C01-120613	1
Caelo	Progesterone	EU-HTT160708	1
Caelo	Progesterone	EU-HTT180317	1
Caelo	Progesterone	HTT140302	1
Caeolo/Gehe	Progesterone	17060903	2
Caesar & Loretz GmbH...	Progesterone	18263804	1
Caesar & Loretz GmbH...	Progesterone	21001388003	1
Caesar & Loretz GmbH...	Progesterone	182638010	1
Caesar & Loretz GmbH...	Progesterone	21001388003	1
Caesar & Loretz GmbH/Gehe	Progesterone	18263801	1
Caesar & Loretz GmbH/Gehe	Progesterone	18263809	1
Caesar & Loretz GmbH...	Progesterone	18263804	1
Caesar & Loretz GmbH...	Progesterone	18263804	1
Caesar & Loretz GmbH...	Progesterone	18263809	2
Caesar & Loretz GmbH...	Progesterone	19128705	4
Caesar & Loretz GmbH...	Progesterone	20004530002	1
Caesar & Loretz GmbH/phö	Progesterone	182638004	1
Caesar & Loretz GmbH...	Progesterone	21001388003	1
Caesar & Loretz GmbH	Progesterone	17060910	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Progesterone	17348404	1
Caesar & Loretz GmbH	Progesterone	17348405	1
Caesar & Loretz GmbH	Progesterone	17348409	2
Caesar & Loretz GmbH	Progesterone	182638004	5
Caesar & Loretz GmbH	Progesterone	182638010	9
Caesar & Loretz GmbH	Progesterone	18263804	6
Caesar & Loretz GmbH	Progesterone	18263807	3
Caesar & Loretz GmbH	Progesterone	18263809	5
Caesar & Loretz GmbH	Progesterone	20004530002	4
Caesar & Loretz GmbH	Progesterone	2007029-01	1
Caesar & Loretz GmbH	Progesterone	21001388001	3
Caesar & Loretz GmbH	Progesterone	21001388003	2
Caesar & Loretz GmbH	Progesterone	21001388004	4
Caesar & Loretz GmbH	Progesterone	21001388007	2
Caesar & Loretz GmbH	Progesterone	21001388011	1
Caesar & Loretz GmbH	Progesterone	22001580001	3
Caesar & Loretz GmbH	Progesterone	23002143003	1
Caesar & Loretz GmbH	Progesterone	EUHTT190101	1
Caesar & Loretz/Geil...	Progesterone	17060904	1
Caesar & Loretz/Noweda	Progesterone	19000591004	3
Caesar u Loretz	Progesterone	13155920	1
Caesar u Loretz	Progesterone	15124919	1
Caesar&Lorenz	Progesterone	16103605	1
Caesar/Noweda	Progesterone	12195912	1
Cealo/Noweda	Progesterone	16103607	1
Changzhou Jiaerke Pharma	Progesterone	1308015-01	1
China Medica	Progesterone	1308015-01	1
Ebert u. Jacobi 1...	Progesterone	15C31-B06-312963	1
Ebert-Jacobi	Progesterone	16J05-B04-328263	1
EuRho/EuRho	Progesterone	1904033-01	1
EuRho	Progesterone	1304040-02	1
euRho	Progesterone	2103020-01	1
EuRho	Progesterone	2203007-01	1
Euro OTC	Progesterone		2
Euro OTC	Progesterone	1111053-01	6
Euro OTC	Progesterone	1206024-01	1
Euro OTC	Progesterone	1211004-01	5
Euro OTC	Progesterone	12195924	1
Euro OTC	Progesterone	130404001	1
Euro OTC	Progesterone	1304040-01	4
Euro OTC	Progesterone	1304040-02	3
Euro OTC	Progesterone	1308015-01	3
Euro OTC	Progesterone	1401002-01	3
Euro OTC	Progesterone	1403019-01	2
Euro OTC	Progesterone	1406022-01	1
Euro OTC	Progesterone	140602202	1
Euro OTC	Progesterone	1406022-02	2
Euro OTC	Progesterone	1406910-01	1
Euro OTC	Progesterone	1409019-01	1
Euro OTC	Progesterone	1409029-01	6
Euro OTC	Progesterone	1409029-1	1
Euro OTC	Progesterone	140910-01	1
Euro OTC	Progesterone	141104301	1
Euro OTC	Progesterone	1411043-01	4
Euro OTC	Progesterone	15/11-B05-315224	1
Euro OTC	Progesterone	1502030-01	2
Euro OTC	Progesterone	1503012-01	7
Euro OTC	Progesterone	1503033-01	1
Euro OTC	Progesterone	1506033-01	51
Euro OTC	Progesterone	1509008_01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Progesterone	1509008-01	7
Euro OTC	Progesterone	1509008-02	31
Euro OTC	Progesterone	160100901	1
Euro OTC	Progesterone	1601009-01	55
Euro OTC	Progesterone	1601009-02	52
Euro OTC	Progesterone	1603004-01	46
Euro OTC	Progesterone	1603012-01	1
Euro OTC	Progesterone	1605013-01	35
Euro OTC	Progesterone	1605013-02	45
Euro OTC	Progesterone	160501303	2
Euro OTC	Progesterone	1605013-03	6
Euro OTC	Progesterone	1605032-01	46
Euro OTC	Progesterone	160532-01	15
Euro OTC	Progesterone	1609001-01	65
Euro OTC	Progesterone	1701038-01	30
Euro OTC	Progesterone	170103802	9
Euro OTC	Progesterone	1701038-02	33
Euro OTC	Progesterone	170138-01	20
Euro OTC	Progesterone	1704012-01	8
Euro OTC	Progesterone	1705028	1
Euro OTC	Progesterone	170502801	1
Euro OTC	Progesterone	1705028-01	64
Euro OTC	Progesterone	1706009-01	9
Euro OTC	Progesterone	1709012-01	100
Euro OTC	Progesterone	17I08-B04	1
Euro OTC	Progesterone	1801036-01	11
Euro OTC	Progesterone	1801036-02	16
Euro OTC	Progesterone	18041816	1
Euro OTC	Progesterone	1806020-01	55
Euro OTC	Progesterone	1806020-02	1
Euro OTC	Progesterone	180901701	20
Euro OTC	Progesterone	1809017-01	62
Euro OTC	Progesterone	1809017-02	1
Euro OTC	Progesterone	1809018-02	1
Euro OTC	Progesterone	1811033-01	64
Euro OTC	Progesterone	1901021-01	3
Euro OTC	Progesterone	1901022-01	36
Euro OTC	Progesterone	1904033_01	1
Euro OTC	Progesterone	1904033-01	6
Euro OTC	Progesterone	190433-01	1
Euro OTC	Progesterone	1905022-01	4
Euro OTC	Progesterone	1905023-01	3
Euro OTC	Progesterone	1908002-01	12
Euro OTC	Progesterone	1908003-01	3
Euro OTC	Progesterone	1911006-01	1
Euro OTC	Progesterone	1911007-01	38
Euro OTC	Progesterone	19A25-B01-360449	1
Euro OTC	Progesterone	2001036-01	1
Euro OTC	Progesterone	2003036-01	2
Euro OTC	Progesterone	2003037-01	1
Euro OTC	Progesterone	2003042	2
Euro OTC	Progesterone	200304201	2
Euro OTC	Progesterone	2003042-01	1
Euro OTC	Progesterone	2005018-01	4
Euro OTC	Progesterone	2005019-01	19
Euro OTC	Progesterone	2006017-02	3
Euro OTC	Progesterone	2006018-01	95
Euro OTC	Progesterone	200618-01	1
Euro OTC	Progesterone	2007028-02	3
Euro OTC	Progesterone	2007029-01	122

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Progesterone	2010005-01	56
Euro OTC	Progesterone	2103019-01	3
Euro OTC	Progesterone	2103020-01	106
Euro OTC	Progesterone	210801001	1
Euro OTC	Progesterone	2108010-01	97
Euro OTC	Progesterone	2108011-01	3
Euro OTC	Progesterone	2111008-01	3
Euro OTC	Progesterone	2111009-01	5
Euro OTC	Progesterone	2203006-01	3
Euro OTC	Progesterone	2203007-01	7
Euro OTC	Progesterone	2210016-01	1
Euro OTC	Progesterone	2210017	1
Euro OTC	Progesterone	2210017-01	1
Euro OTC	Progesterone	27061713	1
Euro OTC	Progesterone	5102	1
Euro OTC	Progesterone	5104	1
Euro OTC	Progesterone	7406022-01	1
Euro OTC	Progesterone	818A-03235	1
Euro OTC	Progesterone	c01-111218	1
Euro OTC	Progesterone	c01-130301	1
Euro OTC	Progesterone	C01-130301(M)	2
Euro OTC	Progesterone	C01-130301M	1
Euro OTC	Progesterone	co1-111218(M)	1
Euro OTC	Progesterone	EuroOTC	1
Euro OTC	Progesterone	HTT160102	1
Euro/ Sanacorp	Progesterone	C01-131116(M)	1
EURO/Noweda	Progesterone	191100701	1
EURO/Noweda	Progesterone	200304201	1
Euro	Progesterone	1509008-02	1
Europh-Jenne	Progesterone	1406022-01	1
Fagron	Progesterone		2
Fagron	Progesterone	1-111218	1
Fagron	Progesterone	12A19-N04	1
Fagron	Progesterone	12D05-N06	3
Fagron	Progesterone	12G05-N17	6
Fagron	Progesterone	12K05-N01	2
Fagron	Progesterone	12k05-n07	1
Fagron	Progesterone	12K05-N07	1
Fagron	Progesterone	13/11-N11	1
Fagron	Progesterone	1311-N11	1
Fagron	Progesterone	13A02N01	1
Fagron	Progesterone	13A02-N01	3
Fagron	Progesterone	13AC2-N01	1
Fagron	Progesterone	13b08-n01	1
Fagron	Progesterone	13G11-N02	6
Fagron	Progesterone	13h01-n03	1
Fagron	Progesterone	13H01-N03	7
Fagron	Progesterone	13I11-N11	2
Fagron	Progesterone	13k28-b30-288261	1
Fagron	Progesterone	13K28-B30-288261	1
Fagron	Progesterone	13K28-B30-288262	1
Fagron	Progesterone	13K-B30-288261	1
Fagron	Progesterone	14C10-B01	1
Fagron	Progesterone	14C10B0129347	1
Fagron	Progesterone	14c10-b01-293478	1
Fagron	Progesterone	14c10-B01-293478	1
Fagron	Progesterone	14C10-B01-293478	2
Fagron	Progesterone	14D22-B04	2
Fagron	Progesterone	14D22B04293476	1
Fagron	Progesterone	14D22-B04-293476	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Progesterone	14D22-B04-293477	1
Fagron	Progesterone	14D22-B293479	1
Fagron	Progesterone	14D22-Bo4	1
Fagron	Progesterone	14H13-B05-300216	7
Fagron	Progesterone	14k11-b04	1
Fagron	Progesterone	14K11-B04	3
Fagron	Progesterone	14K11-B04_300921	1
Fagron	Progesterone	14K11-B04-3000920	1
Fagron	Progesterone	14K11B04300920	1
Fagron	Progesterone	14K11-B04-300920	6
Fagron	Progesterone	14K11-B04-300921	3
Fagron	Progesterone	14L15-B05-302292	2
Fagron	Progesterone	14O22-B04-293476	1
Fagron	Progesterone	15/11-B05-315224	3
Fagron	Progesterone	1511-805	1
Fagron	Progesterone	1511-B05-313598	2
Fagron	Progesterone	1511-B05-313598GB	1
Fagron	Progesterone	1511-B05-314184	1
Fagron	Progesterone	1511-B05-314842	1
Fagron	Progesterone	1511B05-315224	1
Fagron	Progesterone	15B12-B04-304837	2
Fagron	Progesterone	15B12-Bo4-304838	1
Fagron	Progesterone	15C31-B06	3
Fagron	Progesterone	15C31B06308439	1
Fagron	Progesterone	15C31-B06-308439	7
Fagron	Progesterone	15C31-B06-308786	1
Fagron	Progesterone	15C31-B06-308796	4
Fagron	Progesterone	15C31-B06-309790	3
Fagron	Progesterone	15C31-B06-312963	1
Fagron	Progesterone	15C31-B06-313599	1
Fagron	Progesterone	15C31-B06-316105	3
Fagron	Progesterone	15C31-Bo6-308796	1
Fagron	Progesterone	15I11-B05	1
Fagron	Progesterone	15I11-B05-313598	2
Fagron	Progesterone	15I11-B05-314184	4
Fagron	Progesterone	15I11-B05-314842	1
Fagron	Progesterone	15I11-B05-315224	3
Fagron	Progesterone	1605013-03	1
Fagron	Progesterone	160A20-B02-321373	1
Fagron	Progesterone	16a20-b02-318667	1
Fagron	Progesterone	16A20-B02-318667	3
Fagron	Progesterone	16A20-B02-318668	1
Fagron	Progesterone	16A20-B02-319103	2
Fagron	Progesterone	16A20-B02-321373	2
Fagron	Progesterone	16A20-B02-321374	4
Fagron	Progesterone	16a20-b02-321375	1
Fagron	Progesterone	16A20-B02-321375	2
Fagron	Progesterone	16D13-B04-323636	1
Fagron	Progesterone	16g115-b04-325136	1
Fagron	Progesterone	16g15-b04	1
Fagron	Progesterone	16G15-B04	2
Fagron	Progesterone	16G15-B04-325135	1
Fagron	Progesterone	16G15-B04325136	1
Fagron	Progesterone	16G15-B04-325136	4
Fagron	Progesterone	16G15B04-325279	1
Fagron	Progesterone	16G15-B04325279	1
Fagron	Progesterone	16G15-B04-325279	6
Fagron	Progesterone	16G15-B04-325755	4
Fagron	Progesterone	16G15-B04-32579	1
Fagron	Progesterone	16g15-b04-326487	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Progesterone	16G15-B04-326487	3
Fagron	Progesterone	16J05-B04-328263	3
Fagron	Progesterone	16J05-B04-328303	3
Fagron	Progesterone	16l11-B04-314184	1
Fagron	Progesterone	16L29-B03	1
Fagron	Progesterone	16L29-B03-302060	1
Fagron	Progesterone	16L29-B03-330995	2
Fagron	Progesterone	16l29b03332060	1
Fagron	Progesterone	16L29-B03-332060	5
Fagron	Progesterone	16L29-B03-332505	4
Fagron	Progesterone	16L29-B-332061	1
Fagron	Progesterone	17/21-B03-341517	1
Fagron	Progesterone	17/21-B03-341518	1
Fagron	Progesterone	17/21-B03-342134	2
Fagron	Progesterone	17/21-B03-342135	2
Fagron	Progesterone	17/21-B03-343284	2
Fagron	Progesterone	17060911	1
Fagron	Progesterone	1721B03342134	1
Fagron	Progesterone	1721-B03-342136	1
Fagron	Progesterone	17C15-B03	1
Fagron	Progesterone	17C15B03333671	2
Fagron	Progesterone	17C15-B03-333671	3
Fagron	Progesterone	17C15-B03-333671	1
Fagron	Progesterone	17C15-B03-333672	2
Fagron	Progesterone	17d25-b06	1
Fagron	Progesterone	17D25-B06-339651	3
Fagron	Progesterone	17D25-B06-339655	2
Fagron	Progesterone	17I08-B04	1
Fagron	Progesterone	17I08-B04-344773	1
Fagron	Progesterone	17I21-803	1
Fagron	Progesterone	17I21-B03	1
Fagron	Progesterone	17I21-B03-341516	2
Fagron	Progesterone	17I21-B03-341518	2
Fagron	Progesterone	17I21-B03-341520	3
Fagron	Progesterone	17I21-B03-342135	1
Fagron	Progesterone	17I21-B03-343284	2
Fagron	Progesterone	18806-B10-349153	1
Fagron	Progesterone	18B06_B10_349775	1
Fagron	Progesterone	18B06-B10	5
Fagron	Progesterone	18B06-B10-346701	5
Fagron	Progesterone	18B06-B10-346702	2
Fagron	Progesterone	18B06-B10-346704	4
Fagron	Progesterone	18B06B10347484	1
Fagron	Progesterone	18B06-B10-347484	4
Fagron	Progesterone	18B06-B10-349153	1
Fagron	Progesterone	18B06-B10-349775	3
Fagron	Progesterone	18F22_B04_354899	1
Fagron	Progesterone	18F22-B04	5
Fagron	Progesterone	18F-22-B04	1
Fagron	Progesterone	18F22-B04-351145	3
Fagron	Progesterone	18F22-B04-351435	3
Fagron	Progesterone	18F22-B04-351998	2
Fagron	Progesterone	18F22-B04-352735	3
Fagron	Progesterone	18F22-B04-352736	1
Fagron	Progesterone	18f22-B04-353582	1
Fagron	Progesterone	18F22-B04-353582	2
Fagron	Progesterone	18F22-B04353582-P201	1
Fagron	Progesterone	18F22-B04-354899	3
Fagron	Progesterone	18F22-B04-354900	4
Fagron	Progesterone	18F22-B04-354901	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Progesterone	18F22-B04-355395	7
Fagron	Progesterone	18F22-HTT180317	1
Fagron	Progesterone	1910213235	1
Fagron	Progesterone	19A25-B01	1
Fagron	Progesterone	19A25-B01-360448	1
Fagron	Progesterone	19A25-B01-360449	5
Fagron	Progesterone	19A25-B01-360450	1
Fagron	Progesterone	19A25-B01-360452	1
Fagron	Progesterone	19A25-B01-360458	3
Fagron	Progesterone	19H20-F02	9
Fagron	Progesterone	19H20-F02-364866	3
Fagron	Progesterone	19H20-F02-364867	2
Fagron	Progesterone	19H20-F02-364868	4
Fagron	Progesterone	19H20-F02-364869	2
Fagron	Progesterone	19H20-F02-364870	2
Fagron	Progesterone	19H20-F02-364871	1
Fagron	Progesterone	19H2O-F02-364866	1
Fagron	Progesterone	19J22-F05	2
Fagron	Progesterone	19J22-F05-3655503	1
Fagron	Progesterone	19J22F05-365551	1
Fagron	Progesterone	19J22-F05-365551	3
Fagron	Progesterone	19J22-F05-365552	4
Fagron	Progesterone	19J22-F05-365553	7
Fagron	Progesterone	19J22-F05-365555	1
Fagron	Progesterone	19J22-F05-365556	2
Fagron	Progesterone	19K11-F04	3
Fagron	Progesterone	19K11-F04-3660209	1
Fagron	Progesterone	19K11-F04-366029	2
Fagron	Progesterone	19K11-F04-366031	1
Fagron	Progesterone	19K11-F04-366033	2
Fagron	Progesterone	200650-0003	1
Fagron	Progesterone	200650-0004	2
Fagron	Progesterone	200650-315224	1
Fagron	Progesterone	20103-F01-374019	1
Fagron	Progesterone	20103-F01-374023	1
Fagron	Progesterone	20103-F01-375531	1
Fagron	Progesterone	20170427Ma6	1
Fagron	Progesterone	20F18-F12	3
Fagron	Progesterone	20F18-F12-32269	1
Fagron	Progesterone	20F18-F12-3722607	1
Fagron	Progesterone	20F18-F12-372267	3
Fagron	Progesterone	20F18-F12-372268	2
Fagron	Progesterone	20F18-f12-372269	1
Fagron	Progesterone	20F18-F12-372269	1
Fagron	Progesterone	20F18-F12-372270	9
Fagron	Progesterone	20F18-F12-372271	1
Fagron	Progesterone	20F18-F12-372272	6
Fagron	Progesterone	20F18-F12-372274	1
Fagron	Progesterone	20F18-F12-372275	3
Fagron	Progesterone	20I03-F01-374018	4
Fagron	Progesterone	20I03-F01-374019	2
Fagron	Progesterone	20I03-F01-374023	2
Fagron	Progesterone	20i03F01375531	1
Fagron	Progesterone	20I03-F01-375531	1
Fagron	Progesterone	21E11-F01	1
Fagron	Progesterone	21E11-F01-378406	2
Fagron	Progesterone	21F01-F02-378515	1
Fagron	Progesterone	21G14F04	1
Fagron	Progesterone	21G14-F04	2
Fagron	Progesterone	21G14-F04-379182	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Progesterone	21G14-F04-379183	9
Fagron	Progesterone	21G14-F04-379607	2
Fagron	Progesterone	21G14-F04-379608	1
Fagron	Progesterone	21G14-F04-381038	1
Fagron	Progesterone	21G14-F04-379607	1
Fagron	Progesterone	22A31-F02	1
Fagron	Progesterone	22A31-F02-381709	1
Fagron	Progesterone	22A31-F02-381711	2
Fagron	Progesterone	22A31-F02-381712	1
Fagron	Progesterone	22A31-F02-381713	1
Fagron	Progesterone	22A31-F02-381714	5
Fagron	Progesterone	22D05-F03-382185	1
Fagron	Progesterone	22H12-B01	4
Fagron	Progesterone	22H12-B02-226405	1
Fagron	Progesterone	22H12-Bo1	1
Fagron	Progesterone	23B08_B03_227303	1
Fagron	Progesterone	23B08-B03-227300	1
Fagron	Progesterone	23B08-B03-227303	2
Fagron	Progesterone	23H07-B04-232935	1
Fagron	Progesterone	375779	1
Fagron	Progesterone	5013I-03235	1
Fagron	Progesterone	ApC01-180128P	1
Fagron	Progesterone	C01-120322	1
Fagron	Progesterone	C01-130301	1
Fagron	Progesterone	C01-170814	1
Fagron	Progesterone	C01-171216	1
Fagron	Progesterone	EU_HTT190405	1
Fagron	Progesterone	EU-HTT160502	1
Fagron	Progesterone	EU-HTT160705	2
Fagron	Progesterone	EU-HTT180317	1
Fagron	Progesterone	EU-HTT190101	1
Fagron	Progesterone	EU-HTT190405	1
Fagron	Progesterone	EU-HTT200401	3
Fagron	Progesterone	EU-HTT220202M	1
Fagron	Progesterone	EU-HTT220316M	1
Fagron	Progesterone	F01-3740202	1
Fagron	Progesterone	F01-3740203	2
Fagron	Progesterone	F01-3755301	1
Fagron	Progesterone	F02-3648606	1
Fagron	Progesterone	F05_3655501	1
Fagron	Progesterone	F05-3655505	1
Fagron	Progesterone	F12-3722607	3
Fagron	Progesterone	F12-3722609	2
Fagron	Progesterone	F12-3722700	1
Fagron	Progesterone	F12-3722702	1
Fagron	Progesterone	F12-3722704	2
Fagron	Progesterone	F12-372271	1
Fagron	Progesterone	HTT140207	1
Fagron	Progesterone	HTT140302	1
Fagron	Progesterone	HTT140413	1
Fagron	Progesterone	HTT140503	1
Fagron	Progesterone	HTT140903	1
Fagron	Progesterone	HTT150201	3
Fagron	Progesterone	intern20180619Ma3	1
Fargon	Progesterone	16L29-B03-332505	1
fargon	Progesterone	18I03-B02-355396	1
Fargon	Progesterone	19J22-F-05-365555	1
Fiebig	Progesterone	17060909	1
Fiebig	Progesterone	17I21-B03	1
Fragon	Progesterone	13A02-N02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
fragron	Progesterone	16A20-B02-319103	1
Gehe	Progesterone	15319608	1
Gehe	Progesterone	17060903	1
Gehe	Progesterone	18B06-B10-347484	1
Gehe	Progesterone	2309026-02	1
Geilenkirchen	Progesterone	16103605	1
Geilenkirchen	Progesterone	16103614	1
Geilenkirchen	Progesterone	17060904	2
Geilenkirchen	Progesterone	17060909	1
Geilenkirchen	Progesterone	17348407	2
Hubei Gedian Humanwell	Progesterone	EU-HTT200401	1
keine Angabe	Progesterone	1304040-01	2
Klenk	Progesterone	C01-120322	1
Kögl	Progesterone	1802398	1
L12	Progesterone	1605013-01	1
L12	Progesterone	17060909	2
L30	Progesterone	17060910	1
L30	Progesterone	18B06-B10-349775	1
Muster	Progesterone	HTT150801	1
Muster	Progesterone	HTT151101	1
Noweda	Progesterone	18B06-B10-349775	1
Noweda	Progesterone	19K11-F04-366029	1
Noweda	Progesterone	23002143004	1
Noweda	Progesterone	F04-3660209	1
Parthe Apotheke	Progesterone	71/21	1
PHOENIX am 18.03.2014	Progesterone	13A02-N01	1
Phoenix 09.12.14	Progesterone	13H01-N03	1
Phoenix 28.03.2014	Progesterone	13G11-N02	1
Phoenix/Cealo	Progesterone	17/21-B03-341517	1
Phoenix	Progesterone	20F18-F12	1
Phoenix	Progesterone	20F18-F12-372270	1
Phoenix	Progesterone	EU-HTT190405	1
Phönix	Progesterone	13155920	1
Phönix	Progesterone	15319604	1
Phönix	Progesterone	15319620	1
Phönix	Progesterone	1605013-01	1
Phönix	Progesterone	16A20-B02-319103	1
Phönix	Progesterone	16G15-B04_325135	1
phönix	Progesterone	16g15-b04-326487	1
Phönix	Progesterone	2003042-01	1
phönix	Progesterone	20F18-F12-372269	1
Phönix	Progesterone	20F18-F12-372269	1
Phönix	Progesterone	21E11-F013778406	1
Phönix	Progesterone	23002143003	1
Sanacorp Caesar & Lo…	Progesterone	21001388003	2
Sanacorp Verbund	Progesterone	20I03-F01-374020	1
Sanacorp	Progesterone	12195914	1
Sanacorp	Progesterone	12195928	1
Sanacorp	Progesterone	13155902	1
Sanacorp	Progesterone	13A02-N01	1
Sanacorp	Progesterone	14C10-B01-293478	1
Sanacorp	Progesterone	15/11-B05-315224	3
sanacorp	Progesterone	15124902	1
Sanacorp	Progesterone	17D25-B06	1
Sanacorp	Progesterone	1809017-01	1
Sanacorp	Progesterone	19H20-F02-364869	1
Sanacorp	Progesterone	19J22-F05	1
Sanacorp	Progesterone	2007029-01	1
Sanacorp	Progesterone	20F18-F12	2
Sanacorp	Progesterone	21001388015	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Progesterone	2111009-01	1
Sanacorp	Progesterone	23002143003	1
Sanacorp	Progesterone	23H07-B03-230995	1
unbekannt	Progesterone	104704	1
Vdl 28.04.14;Preis 39,95	Progesterone		1
VDL;07.11.14;39,95 euro	Progesterone	13155921	1

- 232 820 spectra from 1515 *Apo-Ident* customers from a total of 48 680 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Progesterone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Progesterone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	906	0	152 056
Type B	0	6386	0	195 698
Type C	0	3201	46	232 820

The substance/substance group *Progesterone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.3377 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.9060 %)
Type C	100.0000 % (> 99.9007 %)	98.5833 % (> 98.4909 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20718	22303	5.19	67.83
21868	21868	0.00	75.89
21870	21870	0.00	72.99
21907	21907	0.00	74.86
22226	22226	0.00	68.88
22301	22301	0.00	76.95
22303	22303	0.00	71.97
22525	22525	0.00	83.57
22830	21907	3.67	83.57
22831	22303	3.75	76.05
23249	22303	5.56	71.74
25273	25273	0.00	71.02
25658	25658	0.00	73.24
25684	25684	0.00	76.02

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Proline**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21034-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Proline; Prolinum

Special notes

When selecting the *Proline* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Proline	9	4	2

Second-stage model

For differentiation of the substance/substance group *Proline* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Proline* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	82.56	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Proline* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Proline*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Proline	1606010	22677	40	20160714*
Euro OTC	Proline	1705021	23546	40	20170720*
Euro OTC	Proline	1801047	23961	40	20180206*
Euro OTC	Proline	2009012	25418	40	20200928*
Euro OTC	Proline	2111021	25916	40	20220112*
Euro OTC	Proline	2205012	26210	40	20220608*
Euro OTC	Proline	2205012	26210SI	20	20220608*
Euro OTC	Proline	2308005	26870	40	20230824*
Euro OTC	Proline	2308005	26870SI	20	20230824*
Fagron	Proline	15D13-B02-308152	22270	60	1704059
Fagron	Proline	16J14-B01-327195	23109	40	20161116

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 420 spectra of 11 reference samples from the substance/substance group *Proline*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 542 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 210 spectra of 6 reference samples from the substance/substance group *Proline*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Proline	L1210046-01	21103	40
Euro OTC	Proline	1606010-01	23013	40
Euro OTC	Proline	1812009	24419	40
Euro OTC	Proline	1909002	24844	40
Euro OTC	Proline	1606010-01	23100	40
Euro OTC	Proline	2111021	25916SI†	10

- 201 874 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2 spectra from 2 *Apo-Ident* customers from 2 batches from the substance/substance group *Proline*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
Euro OTC	Proline	L1210046-03	1
Fagron	Proline	20J01-F13-374496	1

- 236 065 spectra from 1515 *Apo-Ident* customers from a total of 49 256 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Proline* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Proline* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	210	0	201 874
Type C	0	2	0	236 065

The substance/substance group *Proline* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.1429 %)
Type C	100.0000 % (> 99.9013 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22270	22270	0.00	217.10
22677	22677	0.00	176.08
23109	22270	4.64	216.08
23546	23546	0.00	186.65

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23961	23961	0.00	207.89
25418	25418	0.00	216.53
25916	25916	0.00	215.43
26210	26210	0.00	212.72
26870	26870	0.00	212.18

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Propranolol hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20954-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Propranolol hydrochloride; Propranololi hydrochloridum

Special notes

When selecting the *Propranolol hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Propranolol hydrochloride	6	5	197

Second-stage model

For differentiation of the substance/substance group *Propranolol hydrochloride* the following second-stage model is used:

- Submodel 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Propranolol hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	114.73	–
⋮	⋮	⋮
Atropine sulfate	>50	78.49
Mometasone furoate	>50	113.47
Phenytoin	>50	120.34
Saccharin sodium	>50	162.11
Quinoline yellow	>50	225.86
Potassium sorbate	>50	228.46
Magnesium hydrogen citrate	>50	250.79
Hydrocortisone	>50	331.06
Calcium orotate dihydrate	>50	432.33
Escin, water-soluble	>50	620.18

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Propranolol hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Propranolol hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Propranolol hydrochloride	12370712	21396	60	20130116
Caelo	Propranolol hydrochloride	12370712	21410	60	20130116
Caelo	Propranolol hydrochloride	15283302	22590	40	20150929
Fagron	Propranolol hydrochloride	13I13-N04	20954	40	1402307
Fagron	Propranolol hydrochloride	15F16-B02-312979	22591	40	20150630
Fagron	Propranolol hydrochloride	18D23-B09-363591	25174	40	20180525
Fagron	Propranolol hydrochloride	20G30-F01-373061	25483	40	20200828

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 320 spectra of 7 reference samples from the substance/substance group *Propranolol hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Propranolol hydrochloride*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Propranolol hydrochloride	171722	23650	40
Caelo	Propranolol hydrochloride	173330	23836	40
Caelo	Propranolol hydrochloride	192472	24878	40
Caelo	Propranolol hydrochloride	23000119	26718	40
Fagron	Propranolol hydrochloride	23A11-B01-224499	26616	40
Caelo	Propranolol hydrochloride	23000119	26718SI	20
Fagron	Propranolol hydrochloride	23A11-B01-224499	26616SI	20

- 201 844 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1512 spectra from 572 *Apo-Ident* customers from 215 batches from the substance/substance group *Propranolol hydrochloride*.

- Among them are spectra of independent samples from 195 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Propranolol hydrochloride	21002211012	3
	Propranolol hydrochloride	21002211013	2
	Propranolol hydrochloride	21002211014	3
	Propranolol hydrochloride	21002211016	2
	Propranolol hydrochloride	2100221104	1
	Propranolol hydrochloride	2102211012	1
	Propranolol hydrochloride	21J13-F02-380307	2
	Propranolol hydrochloride	21L01-B01-220233	1
	Propranolol hydrochloride	21L01-B01-222417	6
	Propranolol hydrochloride	23000119001	4
	Propranolol hydrochloride	23000119002	17
	Propranolol hydrochloride	2300119002	1
	Propranolol hydrochloride	230019002	1
	Propranolol hydrochloride	23003559002	2
	Propranolol hydrochloride	23E05-B05-229475	10
	Propranolol hydrochloride	23E05-B05-231731	2
	Propranolol hydrochloride	23E05-B05-233780	1
	Propranolol hydrochloride	B01-2241007	1
	Propranolol hydrochloride	B05-2317301	2
	Propranolol hydrochloride	B05-2337800	1
	Propranolol hydrochloride	B05-2378000	1
	Propranolol hydrochloride	M220726	2
/O. Geilenkirchen	Propranolol hydrochloride	15422502	1
1924720008	Propranolol hydrochloride	192472008	2
AHD	Propranolol hydrochloride	15422501	1
AHD	Propranolol hydrochloride	17172204	2
AHD	Propranolol hydrochloride	17333001	1
AHD	Propranolol hydrochloride	17333006	1
AHD	Propranolol hydrochloride	18179402	3
AHD	Propranolol hydrochloride	941895	1
Alliance health	Propranolol hydrochloride	13E15-B40-294297	1
allianz	Propranolol hydrochloride	15283302	1
apomix	Propranolol hydrochloride	15K11-B01-316401	1
Audor Pharma	Propranolol hydrochloride	15K11-B01	1
cae	Propranolol hydrochloride	20003220002	1
Caelo	Propranolol hydrochloride		1
Caelo	Propranolol hydrochloride	12370703	1
Caelo	Propranolol hydrochloride	12370709	1
Caelo	Propranolol hydrochloride	12370710	1
Caelo	Propranolol hydrochloride	12370712	1
Caelo	Propranolol hydrochloride	12a27-n04	1
Caelo	Propranolol hydrochloride	12D27-N14	1
Caelo	Propranolol hydrochloride	13/13-N04	3
Caelo	Propranolol hydrochloride	13379804	1
Caelo	Propranolol hydrochloride	13379806	1
Caelo	Propranolol hydrochloride	13379807	5
Caelo	Propranolol hydrochloride	13379809	3
Caelo	Propranolol hydrochloride	13E15-B40-289355	2
Caelo	Propranolol hydrochloride	13I13N04	1
Caelo	Propranolol hydrochloride	150082405	1
Caelo	Propranolol hydrochloride	15082401	4
Caelo	Propranolol hydrochloride	15082404	1
Caelo	Propranolol hydrochloride	15082405	2
Caelo	Propranolol hydrochloride	15179405	1
Caelo	Propranolol hydrochloride	15283301	13
Caelo	Propranolol hydrochloride	15283302	5
Caelo	Propranolol hydrochloride	154225	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Propranolol hydrochloride	15422501	13
Caelo	Propranolol hydrochloride	15422502	14
Caelo	Propranolol hydrochloride	15422505	7
Caelo	Propranolol hydrochloride	15422505-3032017/2	1
Caelo	Propranolol hydrochloride	1542251	1
Caelo	Propranolol hydrochloride	15F16-B02	1
Caelo	Propranolol hydrochloride	15F16-B02-312979	3
Caelo	Propranolol hydrochloride	15k11-B01	1
Caelo	Propranolol hydrochloride	15K11-B01-316401	1
Caelo	Propranolol hydrochloride	16138302	10
Caelo	Propranolol hydrochloride	16138302-3417/2	1
Caelo	Propranolol hydrochloride	16138304	16
Caelo	Propranolol hydrochloride	16138306	8
Caelo	Propranolol hydrochloride	1616E-03609	1
Caelo	Propranolol hydrochloride	16E09-B09-326637	3
Caelo	Propranolol hydrochloride	16E09-B09-330547	5
Caelo	Propranolol hydrochloride	16E09-B09-333442	1
Caelo	Propranolol hydrochloride	17106PRRII	1
Caelo	Propranolol hydrochloride	1712203	1
Caelo	Propranolol hydrochloride	1712204	1
Caelo	Propranolol hydrochloride	1712205	1
Caelo	Propranolol hydrochloride	17172203	22
Caelo	Propranolol hydrochloride	17172203-20112017/1	1
Caelo	Propranolol hydrochloride	17172204	18
Caelo	Propranolol hydrochloride	17172205	8
Caelo	Propranolol hydrochloride	1733001	1
Caelo	Propranolol hydrochloride	17333001	34
Caelo	Propranolol hydrochloride	173330015654	1
Caelo	Propranolol hydrochloride	17333005	1
Caelo	Propranolol hydrochloride	17333006	13
Caelo	Propranolol hydrochloride	17333008	1
Caelo	Propranolol hydrochloride	1733301	2
Caelo	Propranolol hydrochloride	1733306	1
Caelo	Propranolol hydrochloride	17K22-B03-342731	1
Caelo	Propranolol hydrochloride	17K22-B03-344247	2
Caelo	Propranolol hydrochloride	17K22-B03-345013	4
Caelo	Propranolol hydrochloride	17K22-B03-347251	5
Caelo	Propranolol hydrochloride	18179402	67
Caelo	Propranolol hydrochloride	18179403	34
Caelo	Propranolol hydrochloride	18179405	49
Caelo	Propranolol hydrochloride	18179406	1
Caelo	Propranolol hydrochloride	181799402	1
Caelo	Propranolol hydrochloride	18D23-B09	1
Caelo	Propranolol hydrochloride	18D23-B09-351774	6
Caelo	Propranolol hydrochloride	18D23-B09-355583	6
Caelo	Propranolol hydrochloride	18D23-B09-359713	5
Caelo	Propranolol hydrochloride	19242008	1
Caelo	Propranolol hydrochloride	19247001	1
Caelo	Propranolol hydrochloride	1924720008	1
Caelo	Propranolol hydrochloride	192472001	42
Caelo	Propranolol hydrochloride	192472002	1
Caelo	Propranolol hydrochloride	192472003	41
Caelo	Propranolol hydrochloride	192472008	23
Caelo	Propranolol hydrochloride	19272001	1
Caelo	Propranolol hydrochloride	20003220002	24
Caelo	Propranolol hydrochloride	20003220003	1
Caelo	Propranolol hydrochloride	20003220004	21
Caelo	Propranolol hydrochloride	2000322002	4
Caelo	Propranolol hydrochloride	2000322004	3
Caelo	Propranolol hydrochloride	2003220002	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Propranolol hydrochloride	2003220004	1
Caelo	Propranolol hydrochloride	210002211001	1
Caelo	Propranolol hydrochloride	21002211001	39
Caelo	Propranolol hydrochloride	21002211002	23
Caelo	Propranolol hydrochloride	21002211007	20
Caelo	Propranolol hydrochloride	21002211010	14
Caelo	Propranolol hydrochloride	21002211012	22
Caelo	Propranolol hydrochloride	21002211013	11
Caelo	Propranolol hydrochloride	21002211014	2
Caelo	Propranolol hydrochloride	21002211016	2
Caelo	Propranolol hydrochloride	2100221102	5
Caelo	Propranolol hydrochloride	2100221107	1
Caelo	Propranolol hydrochloride	210507-01	1
Caelo	Propranolol hydrochloride	21052PRRII	1
Caelo	Propranolol hydrochloride	21J13-F02-380307	1
Caelo	Propranolol hydrochloride	23000119002	1
Caelo	Propranolol hydrochloride	2771	1
Caelo	Propranolol hydrochloride	m130104	1
Caelo	Propranolol hydrochloride	M130104	1
Caelo	Propranolol hydrochloride	M141203	1
Caelo	Propranolol hydrochloride	M180207	1
Caeo/Noweda	Propranolol hydrochloride	15283302	1
Caesar & Loretz GmbH…	Propranolol hydrochloride	15422502	1
Caesar & Loretz GmbH…	Propranolol hydrochloride	18179405	1
Caesar & Loretz GmbH…	Propranolol hydrochloride	21002211010	2
Caesar & Loretz GmbH…	Propranolol hydrochloride	18179405	1
Caesar & Loretz GmbH…	Propranolol hydrochloride	192472003	1
Caesar & Loretz GmbH…	Propranolol hydrochloride	20003220002	1
Caesar & Loretz GmbH…	Propranolol hydrochloride	20003220004	2
Caesar & Loretz GmbH…	Propranolol hydrochloride	18179403	5
Caesar & Loretz GmbH…	Propranolol hydrochloride	192472008	1
Caesar & Loretz GmbH/Gehe	Propranolol hydrochloride	20003220002	2
Caesar & Loretz GmbH/Gehe	Propranolol hydrochloride	21002211001	2
Caesar & Loretz GmbH/Gehe	Propranolol hydrochloride	21002211010	2
Caesar & Loretz GmbH/Gehe	Propranolol hydrochloride	21002211012	1
Caesar & Loretz GmbH…	Propranolol hydrochloride	20003220002	2
Caesar & Loretz GmbH/Kehr	Propranolol hydrochloride	18179402	1
Caesar & Loretz GmbH/Kehr	Propranolol hydrochloride	18179405	1
Caesar & Loretz GmbH/Kehr	Propranolol hydrochloride	192472001	1
Caesar & Loretz GmbH/Kehr	Propranolol hydrochloride	21002211013	1
Caesar & Loretz GmbH…	Propranolol hydrochloride	18179402	1
Caesar & Loretz GmbH…	Propranolol hydrochloride	18179403	1
Caesar & Loretz GmbH/Otto	Propranolol hydrochloride	192472001	1
Caesar & Loretz GmbH/Otto	Propranolol hydrochloride	192472008	1
Caesar & Loretz GmbH/P	Propranolol hydrochloride	192472001	2
Caesar & Loretz GmbH…	Propranolol hydrochloride	192472001	3
Caesar & Loretz GmbH…	Propranolol hydrochloride	192472001	1
Caesar & Loretz GmbH…	Propranolol hydrochloride	192472003	1
Caesar & Loretz GmbH…	Propranolol hydrochloride	192472008	1
Caesar & Loretz GmbH…	Propranolol hydrochloride	21002211002	1
Caesar & Loretz GmbH…	Propranolol hydrochloride	20003220002	1
Caesar & Loretz GmbH…	Propranolol hydrochloride	20003220004	1
Caesar & Loretz GmbH…	Propranolol hydrochloride	21002211001	1
Caesar & Loretz GmbH…	Propranolol hydrochloride	21002211012	1
Caesar & Loretz GmbH	Propranolol hydrochloride		1
Caesar & Loretz GmbH	Propranolol hydrochloride	18179402	7
Caesar & Loretz GmbH	Propranolol hydrochloride	18179403	10
Caesar & Loretz GmbH	Propranolol hydrochloride	18179405	17
Caesar & Loretz GmbH	Propranolol hydrochloride	19247001	1
Caesar & Loretz GmbH	Propranolol hydrochloride	192472001	9

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Propranolol hydrochloride	192472003	11
Caesar & Loretz GmbH	Propranolol hydrochloride	192472008	19
Caesar & Loretz GmbH	Propranolol hydrochloride	20003220002	12
Caesar & Loretz GmbH	Propranolol hydrochloride	20003220004	10
Caesar & Loretz GmbH	Propranolol hydrochloride	21002211001	16
Caesar & Loretz GmbH	Propranolol hydrochloride	21002211002	7
Caesar & Loretz GmbH	Propranolol hydrochloride	21002211007	15
Caesar & Loretz GmbH	Propranolol hydrochloride	21002211010	4
Caesar & Loretz GmbH	Propranolol hydrochloride	21002211012	12
Caesar & Loretz GmbH	Propranolol hydrochloride	21002211013	1
Caesar & Loretz GmbH	Propranolol hydrochloride	21002211014	2
Caesar & Loretz GmbH	Propranolol hydrochloride	21002211016	1
Caesar & Loretz GmbH	Propranolol hydrochloride	M180207	3
Caesar u Loretz	Propranolol hydrochloride	13379807	1
Caesar&Loretz GmbH	Propranolol hydrochloride	18179405	1
Caleo	Propranolol hydrochloride	192472008	1
Calo/AHD	Propranolol hydrochloride	15082401	1
Caselo	Propranolol hydrochloride	18179405	1
Cealo, GEHE	Propranolol hydrochloride	20003220002	1
Changhzhou Yabang Ph...	Propranolol hydrochloride	20G30-F01-373061	1
Changzhou / Faron	Propranolol hydrochloride	M151204	1
Changzhou / Gehe	Propranolol hydrochloride	M140808	1
Changzhou Yabang Pha...	Propranolol hydrochloride	15F16-B02	1
Euro OTC	Propranolol hydrochloride	13379806	1
Euro OTC	Propranolol hydrochloride	13I13-N04	1
Euro OTC	Propranolol hydrochloride	15K11B01-320607	1
Euro OTC	Propranolol hydrochloride	15K11-B01-322717	1
Euro OTC	Propranolol hydrochloride	16138304	2
Fagron	Propranolol hydrochloride		2
Fagron	Propranolol hydrochloride	10L20N08	2
Fagron	Propranolol hydrochloride	11D01-N11	1
Fagron	Propranolol hydrochloride	11I19-N09	1
Fagron	Propranolol hydrochloride	11L01-N05	2
Fagron	Propranolol hydrochloride	12A27-N04	1
Fagron	Propranolol hydrochloride	12D27-N14	4
Fagron	Propranolol hydrochloride	12F29-N06	4
Fagron	Propranolol hydrochloride	12F29-NO6	1
Fagron	Propranolol hydrochloride	12K06N07	1
Fagron	Propranolol hydrochloride	12K06-N07	7
Fagron	Propranolol hydrochloride	13/13-N04	4
Fagron	Propranolol hydrochloride	1313-N04	2
Fagron	Propranolol hydrochloride	13E15_B40-297021	1
Fagron	Propranolol hydrochloride	13E15-B40	5
Fagron	Propranolol hydrochloride	13E15-B40-289355	12
Fagron	Propranolol hydrochloride	13E15-B40-294297	5
Fagron	Propranolol hydrochloride	13E15-B40-297021	6
Fagron	Propranolol hydrochloride	13I13-N04	9
Fagron	Propranolol hydrochloride	13J13-N04	3
Fagron	Propranolol hydrochloride	13l13-N04	1
Fagron	Propranolol hydrochloride	15F16-B02	1
Fagron	Propranolol hydrochloride	15F16B02312979	1
Fagron	Propranolol hydrochloride	15F16-B02-312979	4
Fagron	Propranolol hydrochloride	15K11_B01_322717	1
Fagron	Propranolol hydrochloride	15K11-B01	4
Fagron	Propranolol hydrochloride	15K11-B01_320607	1
Fagron	Propranolol hydrochloride	15K11-B01-16401	1
Fagron	Propranolol hydrochloride	15K11-B01-316401	12
Fagron	Propranolol hydrochloride	15K11-B01-320607	8
Fagron	Propranolol hydrochloride	15K11-B01-322717	4
Fagron	Propranolol hydrochloride	15K11-Bo1-316401	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Propranolol hydrochloride	16138302	1
Fagron	Propranolol hydrochloride	16E09-B09	3
Fagron	Propranolol hydrochloride	16E09-B09-326637	16
Fagron	Propranolol hydrochloride	16E09B09330547	1
Fagron	Propranolol hydrochloride	16E09-B09-330547	7
Fagron	Propranolol hydrochloride	16E09-B09333442	1
Fagron	Propranolol hydrochloride	16E09-B09-333442	14
Fagron	Propranolol hydrochloride	17333001	1
Fagron	Propranolol hydrochloride	17K22-B03	5
Fagron	Propranolol hydrochloride	17K22-B03_347251	1
Fagron	Propranolol hydrochloride	17K22-B03-30048	1
Fagron	Propranolol hydrochloride	17k22-B03-342731	2
Fagron	Propranolol hydrochloride	17K22-B03-342731	8
Fagron	Propranolol hydrochloride	17K22-B03-344247	4
Fagron	Propranolol hydrochloride	17K22-B03-345013	1
Fagron	Propranolol hydrochloride	17K-22-B03-345013	1
Fagron	Propranolol hydrochloride	17k22-b03-347251	1
Fagron	Propranolol hydrochloride	17K22-B03-347251	5
Fagron	Propranolol hydrochloride	17K22-b03-350048	1
Fagron	Propranolol hydrochloride	17K22-B03-350048	6
Fagron	Propranolol hydrochloride	18041807	1
Fagron	Propranolol hydrochloride	18D_23-B09-351774	1
Fagron	Propranolol hydrochloride	18D23-B0	1
Fagron	Propranolol hydrochloride	18D23-B09	16
Fagron	Propranolol hydrochloride	18d23b09351774	1
Fagron	Propranolol hydrochloride	18D23-B09-351774	14
Fagron	Propranolol hydrochloride	18D23-B09-3555583	1
Fagron	Propranolol hydrochloride	18D23-B09-355583	10
Fagron	Propranolol hydrochloride	18D23-B09-357778	3
Fagron	Propranolol hydrochloride	18D23-B09-359713	19
Fagron	Propranolol hydrochloride	18D23-B09-363591	8
Fagron	Propranolol hydrochloride	20250711-8	1
Fagron	Propranolol hydrochloride	20G30-F01	4
Fagron	Propranolol hydrochloride	20G30-F01-0001	1
Fagron	Propranolol hydrochloride	20G30-F01-37	1
Fagron	Propranolol hydrochloride	20G30-F01-373060	17
Fagron	Propranolol hydrochloride	20G30-F01-373060/M200409	1
Fagron	Propranolol hydrochloride	20G30-F01-373061	12
Fagron	Propranolol hydrochloride	21J13-F02-380307	15
Fagron	Propranolol hydrochloride	21J3-F02_380307	1
Fagron	Propranolol hydrochloride	21j3-f02-380307	1
Fagron	Propranolol hydrochloride	21L01-B01-220233	1
Fagron	Propranolol hydrochloride	21L01-B01-222417	3
Fagron	Propranolol hydrochloride	23E05-B05-229475	2
Fagron	Propranolol hydrochloride	28051508	1
Fagron	Propranolol hydrochloride	3050PRII	1
Fagron	Propranolol hydrochloride	3050PRRII	2
Fagron	Propranolol hydrochloride	31101201	1
Fagron	Propranolol hydrochloride	3112U-03609	1
Fagron	Propranolol hydrochloride	3913M-03609	1
Fagron	Propranolol hydrochloride	4(20G30-F01-373060)	1
Fagron	Propranolol hydrochloride	402310015	1
Fagron	Propranolol hydrochloride	4071401	1
Fagron	Propranolol hydrochloride	5101	1
Fagron	Propranolol hydrochloride	700556-0001	1
Fagron	Propranolol hydrochloride	8D23-B09-3577781	1
Fagron	Propranolol hydrochloride	9CMK6AA71374	1
Fagron	Propranolol hydrochloride	9L09-N06	1
Fagron	Propranolol hydrochloride	B09-3597103	1
Fagron	Propranolol hydrochloride	B09-3635901	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Propranolol hydrochloride	F01-3730600	2
Fagron	Propranolol hydrochloride	F01-3730601	3
Fagron	Propranolol hydrochloride	M130104	1
Fagron	Propranolol hydrochloride	M141203	1
Fagron	Propranolol hydrochloride	M151204	3
Fagron	Propranolol hydrochloride	M170602	4
Fagron	Propranolol hydrochloride	M180207	6
Fagron	Propranolol hydrochloride	M200409	4
Fagron	Propranolol hydrochloride	M210630	1
Fargon/Noweda	Propranolol hydrochloride	18D23-B09-355583	2
Fargon	Propranolol hydrochloride	12K06-N07	1
Fargon	Propranolol hydrochloride	18D23-B09	1
Fargon	Propranolol hydrochloride	18D23-B09-359713	1
Fargon	Propranolol hydrochloride	M140808	1
Fischar/Alliance Hea...	Propranolol hydrochloride	18D23-B09	2
fragon/AHD	Propranolol hydrochloride	13/13-N04	1
Fragon/Anzag	Propranolol hydrochloride	18D23-B09-359713	1
Gehe Kassel 26.06.2015	Propranolol hydrochloride	15082401	1
Gehe	Propranolol hydrochloride		1
Gehe	Propranolol hydrochloride	16E09-B09	1
Gehe	Propranolol hydrochloride	17172203	1
Gehe	Propranolol hydrochloride	17172205	2
Gehe	Propranolol hydrochloride	18179403	1
GEHE	Propranolol hydrochloride	18179405	1
Gehe	Propranolol hydrochloride	18D23	1
Gehe	Propranolol hydrochloride	192472003	1
Gehe	Propranolol hydrochloride	20003220004	1
Gehe	Propranolol hydrochloride	23000119002	1
Gehe	Propranolol hydrochloride	23E-05-B05-233780	1
Gutenberg-Apotheke	Propranolol hydrochloride	13I13-N04	1
Hedinger, Kehr /07.03.19	Propranolol hydrochloride	18179402	3
Ichthyol-Gesellschaf...	Propranolol hydrochloride	16138302	1
InfectoPharm	Propranolol hydrochloride	J0512011	1
Inresa 22.09.15	Propranolol hydrochloride	3043PRRII	1
IPCA / Noweda	Propranolol hydrochloride	192472003	2
Jenne	Propranolol hydrochloride	17333001	1
JENNE	Propranolol hydrochloride	17333001	1
Jenne	Propranolol hydrochloride	21002211001	2
Jenne	Propranolol hydrochloride	21002211013	1
Kehr	Propranolol hydrochloride	21L01-B01-222417	1
Kehr	Propranolol hydrochloride	23E05-B05-233780	1
Kehr	Propranolol hydrochloride	M180207	1
kontrolle	Propranolol hydrochloride	kontrolleAP210113-01	1
L12	Propranolol hydrochloride	16E09-B09-326637	1
L12	Propranolol hydrochloride	17K22-B03-350048	1
L12	Propranolol hydrochloride	18D23-B09-355583	1
L30	Propranolol hydrochloride	15K11-B01-320607	1
Land IpCA Laboratories	Propranolol hydrochloride	15422502	1
Löwen City-Apotheke ...	Propranolol hydrochloride	4012013	1
Nachprüfung	Propranolol hydrochloride	2082019-1	1
Noweda	Propranolol hydrochloride		1
Noweda	Propranolol hydrochloride	15K11-B01-322717	1
Noweda	Propranolol hydrochloride	17K22-B03-344247	2
Noweda	Propranolol hydrochloride	18179402	2
Noweda	Propranolol hydrochloride	18179405	2
Noweda	Propranolol hydrochloride	18179405/2x	1
Noweda	Propranolol hydrochloride	192472001	1
Noweda	Propranolol hydrochloride	192472008	1
Noweda	Propranolol hydrochloride	20003220002	1
Noweda	Propranolol hydrochloride	20003220004	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Propranolol hydrochloride	2100221002	1
Noweda	Propranolol hydrochloride	21002211012	1
Noweda	Propranolol hydrochloride	23000119002	4
Noweda	Propranolol hydrochloride	23E05-B05-229475	1
Phoenix/Fargron	Propranolol hydrochloride	15K11-B01-322717	2
Phoenix	Propranolol hydrochloride	16138304	1
Phoenix	Propranolol hydrochloride	17K22-B03-344247	1
Phoenix	Propranolol hydrochloride	18179402	1
Phoenix	Propranolol hydrochloride	18D23-B09-355583	1
Phoenix	Propranolol hydrochloride	192472003	1
Phönix/Fragon	Propranolol hydrochloride	18D23-B09-357778	1
Phönix/Fragon	Propranolol hydrochloride	20G30-F01-373060	1
Phönix	Propranolol hydrochloride	15k11-b01-322717	1
Phönix	Propranolol hydrochloride	15k11-B01-322717	1
phönix	Propranolol hydrochloride	16e09-b09	1
phönix	Propranolol hydrochloride	16e09b09326637	1
Phönix	Propranolol hydrochloride	16E09-B09-326637	1
Phönix	Propranolol hydrochloride	17172203	1
Phönix	Propranolol hydrochloride	18179402	1
Phönix	Propranolol hydrochloride	192472003	2
phönix	Propranolol hydrochloride	2/AKD3	1
PHÖNIX	Propranolol hydrochloride	21002211002	1
Sanacorp	Propranolol hydrochloride	12370712	1
Sanacorp	Propranolol hydrochloride	16138304	1
Sanacorp	Propranolol hydrochloride	18D23-B09-351774	1
Sanacorp	Propranolol hydrochloride	20G30-F01	1
Sanacorp	Propranolol hydrochloride	21002211001	1
Sanacorp	Propranolol hydrochloride	23000119002	1
Sanacorp	Propranolol hydrochloride	23E05-B05-229475	1
VDL	Propranolol hydrochloride	18D23-B09-359713	1
WE:Phönix 12.08.2016	Propranolol hydrochloride	15422502	1

- 234 555 spectra from 1515 *Apo-Ident* customers from a total of 49 043 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Propranolol hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Propranolol hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	240	0	201 844
Type C	0	1505	7	234 555

The substance/substance group *Propranolol hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	99.5370 % (> 99.3386 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20954	20954	0.00	235.69
21396	20954	4.29	233.71
21410	20954	21.77	233.80
22590	20954	9.07	234.04
22591	20954	25.34	239.55
25174	20954	34.90	241.04
25483	20954	44.61	241.90

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Propyl-4-hydroxybenzoate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20981-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Propyl-4-hydroxybenzoate; Propylis parahydroxybenzoas

Special notes

When selecting the *Propyl-4-hydroxybenzoate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Propyl-4-hydroxybenzoate	5	3	73

Second-stage model

For differentiation of the substance/substance group *Propyl-4-hydroxybenzoate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Propyl-4-hydroxybenzoate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	92.36	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Propyl-4-hydroxybenzoate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Propyl-4-hydroxybenzoate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Propyl-4-hydroxybenzoate	11373523	20981	40	1402440
Caelo	Propyl-4-hydroxybenzoate	13365009	21758	60	20131203
Caelo	Propyl-4-hydroxybenzoate	162595	22754	40	20161005*
Caelo	Propyl-4-hydroxybenzoate	162595	22765	40	20161005*
Caelo	Propyl-4-hydroxybenzoate	190732	24497	40	20190404*
Caelo	Propyl-4-hydroxybenzoate	22002607	26367	40	20220930*
Caelo	Propyl-4-hydroxybenzoate	22002607	26367SI	20	20220930*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 280 spectra of 7 reference samples from the substance/substance group *Propyl-4-hydroxybenzoate*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 682 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 5 reference samples from the substance/substance group *Propyl-4-hydroxybenzoate*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Propyl-4-hydroxybenzoate	171970	23675	40
Caelo	Propyl-4-hydroxybenzoate	23000158	26708	40
Gatt-Koller	Propyl-4-hydroxybenzoate	22J02745	27098	30
Caelo	Propyl-4-hydroxybenzoate	23000158	26708SI	20
Gatt-Koller	Propyl-4-hydroxybenzoate	22J02745	27098SI	20

- 201 934 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 322 spectra from 236 *Apo-Ident* customers from 76 batches from the substance/substance group *Propyl-4-hydroxybenzoate*.

- Among them are spectra of independent samples from 72 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Propyl-4-hydroxybenzoate	191700004	1
	Propyl-4-hydroxybenzoate	191700004280622/1	1
	Propyl-4-hydroxybenzoate	21000901006	1
	Propyl-4-hydroxybenzoate	21000901013	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
	Propyl-4-hydroxybenzoate	23000158002	9
	Propyl-4-hydroxybenzoate	23000158005	3
AHD	Propyl-4-hydroxybenzoate	11373523	1
Anzag	Propyl-4-hydroxybenzoate	11373512	2
Caelo	Propyl-4-hydroxybenzoate		1
Caelo	Propyl-4-hydroxybenzoate	1108211931	1
Caelo	Propyl-4-hydroxybenzoate	11102609	1
Caelo	Propyl-4-hydroxybenzoate	11102611	2
Caelo	Propyl-4-hydroxybenzoate	11102624	1
Caelo	Propyl-4-hydroxybenzoate	11121709	1
Caelo	Propyl-4-hydroxybenzoate	113735	1
Caelo	Propyl-4-hydroxybenzoate	11373505	1
Caelo	Propyl-4-hydroxybenzoate	11373512	3
Caelo	Propyl-4-hydroxybenzoate	11373518	2
Caelo	Propyl-4-hydroxybenzoate	113735223	1
Caelo	Propyl-4-hydroxybenzoate	11373523	2
Caelo	Propyl-4-hydroxybenzoate	11373524	1
Caelo	Propyl-4-hydroxybenzoate	13051504	1
Caelo	Propyl-4-hydroxybenzoate	13100208	1
Caelo	Propyl-4-hydroxybenzoate	13100215	7
Caelo	Propyl-4-hydroxybenzoate	13100217	3
Caelo	Propyl-4-hydroxybenzoate	13100218	2
Caelo	Propyl-4-hydroxybenzoate	13100219	1
Caelo	Propyl-4-hydroxybenzoate	13365006	5
Caelo	Propyl-4-hydroxybenzoate	13365009	3
Caelo	Propyl-4-hydroxybenzoate	13365011	5
Caelo	Propyl-4-hydroxybenzoate	13365012	2
Caelo	Propyl-4-hydroxybenzoate	14359005	8
Caelo	Propyl-4-hydroxybenzoate	14359006	4
Caelo	Propyl-4-hydroxybenzoate	14359008	26
Caelo	Propyl-4-hydroxybenzoate	14359009	1
Caelo	Propyl-4-hydroxybenzoate	14359019	1
Caelo	Propyl-4-hydroxybenzoate	14359020	4
Caelo	Propyl-4-hydroxybenzoate	14359025	2
Caelo	Propyl-4-hydroxybenzoate	15246501	1
Caelo	Propyl-4-hydroxybenzoate	15246502	2
Caelo	Propyl-4-hydroxybenzoate	15276514	4
Caelo	Propyl-4-hydroxybenzoate	16259505	16
Caelo	Propyl-4-hydroxybenzoate	16259516	16
Caelo	Propyl-4-hydroxybenzoate	16259520	2
Caelo	Propyl-4-hydroxybenzoate	16359006	1
Caelo	Propyl-4-hydroxybenzoate	17343101	12
Caelo	Propyl-4-hydroxybenzoate	17343105	3
Caelo	Propyl-4-hydroxybenzoate	17343108	9
Caelo	Propyl-4-hydroxybenzoate	17343110	8
Caelo	Propyl-4-hydroxybenzoate	19073203	14
Caelo	Propyl-4-hydroxybenzoate	1913I-01931	1
Caelo	Propyl-4-hydroxybenzoate	191700002	1
Caelo	Propyl-4-hydroxybenzoate	191700004	33
Caelo	Propyl-4-hydroxybenzoate	191700007	1
Caelo	Propyl-4-hydroxybenzoate	191700009	3
Caelo	Propyl-4-hydroxybenzoate	19170004	1
Caelo	Propyl-4-hydroxybenzoate	21000601006	1
Caelo	Propyl-4-hydroxybenzoate	21000733001	1
Caelo	Propyl-4-hydroxybenzoate	21000733002	11
Caelo	Propyl-4-hydroxybenzoate	21000901006	2
Caelo	Propyl-4-hydroxybenzoate	220420	1
Caelo	Propyl-4-hydroxybenzoate	221014PAS01	1
Caelo	Propyl-4-hydroxybenzoate	23000158002	2
Caelo	Propyl-4-hydroxybenzoate	290114PML03	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Propyl-4-hydroxybenzoate	3041408	1
Caelo	Propyl-4-hydroxybenzoate	3115M-01931	1
Caelo	Propyl-4-hydroxybenzoate	3217M-01931	1
Caelo	Propyl-4-hydroxybenzoate	4314U-01931	1
Caelo	Propyl-4-hydroxybenzoate	713Q-01931	1
Caelo	Propyl-4-hydroxybenzoate	82792159	1
Caesar & Loretz GmbH...	Propyl-4-hydroxybenzoate	19073203	1
Caesar & Loretz GmbH...	Propyl-4-hydroxybenzoate	19073203	1
Caesar & Loretz GmbH/GEHE	Propyl-4-hydroxybenzoate	17343108	1
Caesar & Loretz GmbH...	Propyl-4-hydroxybenzoate	191700002	1
Caesar & Loretz GmbH...	Propyl-4-hydroxybenzoate	191700004	2
Caesar & Loretz GmbH...	Propyl-4-hydroxybenzoate	17343110	1
Caesar & Loretz GmbH	Propyl-4-hydroxybenzoate	191700004	12
Caesar & Loretz GmbH	Propyl-4-hydroxybenzoate	21000733002	1
Caesar & Loretz GmbH	Propyl-4-hydroxybenzoate	21000733005	1
Caesar & Loretz GmbH	Propyl-4-hydroxybenzoate	21000901006	1
Caesar & Loretz GmbH	Propyl-4-hydroxybenzoate	21000901013	1
Caesar & Loretz GmbHAnzag	Propyl-4-hydroxybenzoate	191700004	1
Caesar & Loretz	Propyl-4-hydroxybenzoate	15276514	1
Caesar &Loretz GmbH	Propyl-4-hydroxybenzoate	13100215	1
Caesar/Noweda	Propyl-4-hydroxybenzoate	3710M-01931	2
Carlo/Phönix/5,95	Propyl-4-hydroxybenzoate	19073203	1
Euro OTC	Propyl-4-hydroxybenzoate	2509025	1
Fagron	Propyl-4-hydroxybenzoate	12B13-N04	1
Fagron	Propyl-4-hydroxybenzoate	610M-01931	1
GATT-KOLLER/PHOENIX	Propyl-4-hydroxybenzoate	5080/11130214	1
Gatt-Koller	Propyl-4-hydroxybenzoate	1800302	1
Gehe 5.3.14	Propyl-4-hydroxybenzoate	13100215	1
Gehe	Propyl-4-hydroxybenzoate	16259505	1
Hänseler	Propyl-4-hydroxybenzoate		1
Kehr	Propyl-4-hydroxybenzoate	23000158002	1
Noweda	Propyl-4-hydroxybenzoate	11373505	1
Noweda	Propyl-4-hydroxybenzoate	14359005	1
Noweda	Propyl-4-hydroxybenzoate	14359020	1
Noweda	Propyl-4-hydroxybenzoate	17343101	1
Noweda	Propyl-4-hydroxybenzoate	17343105	1
PHOENIX 10.03.2014	Propyl-4-hydroxybenzoate	11373526	1
Phoenix	Propyl-4-hydroxybenzoate	13100215	1
Phoenix	Propyl-4-hydroxybenzoate	19073203	1
Phönix 14.01.2014	Propyl-4-hydroxybenzoate	11373526	1
Phönix	Propyl-4-hydroxybenzoate	17343108	1
Sanacorp	Propyl-4-hydroxybenzoate	16259505	1
Sanacorp	Propyl-4-hydroxybenzoate	16259516	1
Sanacorp	Propyl-4-hydroxybenzoate	191700004	1
Sanacorp	Propyl-4-hydroxybenzoate	23000158002	1
Sanacorp	Propyl-4-hydroxybenzoate	23000158005	1
Sanacorp	Propyl-4-hydroxybenzoate	AKD3	1
siehe WE-Prüfprotokoll	Propyl-4-hydroxybenzoate	84/11	1

- 235 745 spectra from 1515 *Apo-Ident* customers from a total of 49 185 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Propyl-4-hydroxybenzoate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this

purpose, all relevant spectra of the various substances were compared with *Propyl-4-hydroxybenzoate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	150	0	201 934
Type C	0	319	3	235 745

The substance/substance group *Propyl-4-hydroxybenzoate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9007 %)	99.0683 % (> 98.1366 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20981	20981	0.00	174.36
21758	26367	11.12	167.75
22754	22754	0.00	184.77
22765	22765	0.00	181.06
24497	24497	0.00	191.42
26367	26367	0.00	181.91

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Propyphenazone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20805-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Propyphenazone; Propyphenazonum

Special notes

When selecting the *Propyphenazone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Propyphenazone	6	4	36

Second-stage model

For differentiation of the substance/substance group *Propyphenazone* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Propyphenazone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Griseofulvin	86.72	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Propyphenazone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Propyphenazone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Propyphenazone	12039103	20805	40	1402051
Caelo	Propyphenazone	13332206	21454	60	20131009
Caelo	Propyphenazone	23000810002	26747	40	20230526
Caelo	Propyphenazone	23000810002	26747SI	20	20230526
Fagron	Propyphenazone	16E02-B08-327928	23261	40	20160602
Fagron	Propyphenazone	16H25-B01-334972	23922	40	20161227
Fagron	Propyphenazone	20C20-B08-202174	25492	40	20200326

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 7 reference samples from the substance/substance group *Propyphenazone*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 682 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 5 reference samples from the substance/substance group *Propyphenazone*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Propyphenazone	15348908	23254	40
Caelo	Propyphenazone	172776	23861	40
Caelo	Propyphenazone	190190	24528	40
Fagron	Propyphenazone	23G05-B08-229442	26904	40
Fagron	Propyphenazone	23G05-B08-229442	26904SI	20

- 201 904 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 83 spectra from 34 *Apo-Ident* customers from 41 batches from the substance/substance group *Propyphenazone*.
- Among them are spectra of independent samples from 36 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Propyphenazone	21000426007	1
Anzag	Propyphenazone	19019003	1
Anzag	Propyphenazone	21000426004	1
Caelo	Propyphenazone	12039101	2
Caelo	Propyphenazone	12039103	1
Caelo	Propyphenazone	12039112	1
Caelo	Propyphenazone	13036702	2
Caelo	Propyphenazone	13137104	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Propyphenazone	13332205	3
Caelo	Propyphenazone	15122502	1
Caelo	Propyphenazone	15122504	3
Caelo	Propyphenazone	15122505	1
Caelo	Propyphenazone	15348901	2
Caelo	Propyphenazone	15348902	2
Caelo	Propyphenazone	15348904	2
Caelo	Propyphenazone	15348908	2
Caelo	Propyphenazone	15348910	1
Caelo	Propyphenazone	15348912	2
Caelo	Propyphenazone	15348913	6
Caelo	Propyphenazone	15348914	2
Caelo	Propyphenazone	17351302	1
Caelo	Propyphenazone	17351304	4
Caelo	Propyphenazone	17351305	1
Caelo	Propyphenazone	190190003	4
Caelo	Propyphenazone	19019003	4
Caesar & Loretz GmbH	Propyphenazone	17351304	1
Caesar & Loretz GmbH	Propyphenazone	21000426002	1
Caleo/Direkt	Propyphenazone	19019003	1
Caleo/Noweda	Propyphenazone	15348913	1
Euro OTC	Propyphenazone		1
Fagron	Propyphenazone	13B12-B02-297171	1
Fagron	Propyphenazone	13K20-B03	2
Fagron	Propyphenazone	13K20-B03-302291	1
Fagron	Propyphenazone	13K20-B03-311715	3
Fagron	Propyphenazone	13k20-b03-319137	1
Fagron	Propyphenazone	13K20B03319137	1
Fagron	Propyphenazone	13K20-B03-319137	3
Fagron	Propyphenazone	13K-B03-319137	1
Fagron	Propyphenazone	16E02-B08-327928	2
Fagron	Propyphenazone	17G03-B01-347588	4
Fagron	Propyphenazone	20A15-B04-196781	1
Fagron	Propyphenazone	20C20-B08-202174	1
Fargon	Propyphenazone	11H31-N07	1
Gatt-Koller / Phoenix	Propyphenazone	419/02123112	1
Gatt-Koller	Propyphenazone	1800011	1
Nachprüfung vom 31.0…	Propyphenazone	13B12-B02-297171	1
Pharmachem	Propyphenazone	15348913	1
Raben-Apotheke Mildenau	Propyphenazone	12039103	1

- 235 984 spectra from 1515 *Apo-Ident* customers from a total of 49 217 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Propyphenazone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Propyphenazone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	180	0	201 904
Type C	0	83	0	235 984

The substance/substance group *Propyphenazone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 92.7711 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20805	20805	0.00	104.38
21454	20805	14.23	103.67
23261	20805	17.45	109.41
23922	20805	24.41	112.27
25492	20805	17.98	106.76
26747	20805	20.68	108.43

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Pyridoxal-5-phosphate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20830-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Pyridoxal-5-phosphate; Pyridoxali phosphas

Special notes

When selecting the *Pyridoxal-5-phosphate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Pyridoxal-5-phosphate	9	5	11

Second-stage model

For differentiation of the substance/substance group *Pyridoxal-5-phosphate* the following second-stage model is used:

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Pyridoxal-5-phosphate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	47.69	–
Silver protein	57.86	–
⋮	⋮	⋮
Sodium citrate	>50	74.58
Levocarnitine	>50	177.40
Capsaicin	>50	190.00
Alfatradiol	>50	204.76
Oxybutynin hydrochloride	>50	208.83
Prednicarbate	>50	322.01
Quinine hydrochloride dihydrate	>50	372.95
Ciprofloxacin hydrochloride	>50	488.59
Tetracaine	>50	488.89
Methoxsalen	>50	493.54
Heparin sodium	>50	523.26
Cyproterone acetate	>50	549.09
Norethisterone acetate	>50	616.47
Amitriptyline hydrochloride	>50	857.06
Valine	>50	1083.81
Triclosan	>50	1127.95
Amifampridine	>50	1335.95
Sucrose	>50	1556.34

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Pyridoxal-5-phosphate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Pyridoxal-5-phosphate*:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Pyridoxal-5-phosphate	1302029-01	20830	40	8897
Euro OTC	Pyridoxal-5-phosphate	1302029-01	21097	40	20130315
Euro OTC	Pyridoxal-5-phosphate	1701015	23133	40	20170220*
Euro OTC	Pyridoxal-5-phosphate	1701015-01	23276	40	20170220
Euro OTC	Pyridoxal-5-phosphate	1808030	24329	40	20181019*
Euro OTC	Pyridoxal-5-phosphate	1902022	24542	40	20190320*
Euro OTC	Pyridoxal-5-phosphate	1908001	24833	40	20190903*
Euro OTC	Pyridoxal-5-phosphate	1910027	24923	40	20191217*
Euro OTC	Pyridoxal-5-phosphate	2102013	25594	40	20210317*
Euro OTC	Pyridoxal-5-phosphate	2104017	25674	40	20210602*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 400 spectra of 10 reference samples from the substance/substance group *Pyridoxal-5-phosphate*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 562 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Pyridoxal-5-phosphate*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Pyridoxal-5-phosphate	1711030	23877	40
Euro OTC	Pyridoxal-5-phosphate	2001043	25130	40
Euro OTC	Pyridoxal-5-phosphate	2003038	25151	40
Euro OTC	Pyridoxal-5-phosphate	2110012	25876	50
Euro OTC	Pyridoxal-5-phosphate	2211016	26589	40
Euro OTC	Pyridoxal-5-phosphate	2110012	25876SI	10
Euro OTC	Pyridoxal-5-phosphate	2211016	26589SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 844 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 27 spectra from 12 *Apo-Ident* customers from 13 batches from the substance/substance group *Pyridoxal-5-phosphate*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Denk	Pyridoxal-5-phosphate	20171202	1
Denk	Pyridoxal-5-phosphate	C041402802	1
EuRho	Pyridoxal-5-phosphate	2003038-01	4
Euro OTC	Pyridoxal-5-phosphate	1701015-01	3
Euro OTC	Pyridoxal-5-phosphate	1711030-01	2
Euro OTC	Pyridoxal-5-phosphate	1808030	1
Euro OTC	Pyridoxal-5-phosphate	1808030-01	2
Euro OTC	Pyridoxal-5-phosphate	1808030-02	4
Euro OTC	Pyridoxal-5-phosphate	1902022-01	1
Euro OTC	Pyridoxal-5-phosphate	1908001-01	4
Euro OTC	Pyridoxal-5-phosphate	2003038-01	1
Euro OTC	Pyridoxal-5-phosphate	2003038-02	1
Fagron	Pyridoxal-5-phosphate	2001043-01	1
Inresa Arznei	Pyridoxal-5-phosphate	13100411	1

- 236 040 spectra from 1515 *Apo-Ident* customers from a total of 49 245 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Pyridoxal-5-phosphate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pyridoxal-5-phosphate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	240	0	201 844
Type C	0	27	0	236 040

The substance/substance group *Pyridoxal-5-phosphate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 77.7778 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20830	20830	0.00	90.72
21097	20830	6.90	84.70
23133	23133	0.00	80.90
23276	20830	14.84	97.14
24329	24329	0.00	164.55
24542	24542	0.00	128.35
24833	24833	0.00	132.18
24923	24923	0.00	146.88
25594	25594	0.00	131.46
25674	25674	0.00	123.68

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Pyridoxine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20440-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Pyridoxine hydrochloride; Pyridoxini hydrochloridum

Special notes

When selecting the *Pyridoxine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Pyridoxine hydrochloride	8	12	60

Second-stage model

For differentiation of the substance/substance group *Pyridoxine hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Pyridoxine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	119.58	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Pyridoxine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Pyridoxine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Pyridoxine hydrochloride	14262302	21675	60	20141002
Caelo	Pyridoxine hydrochloride	162225	22770	40	20160825*
Euro OTC	Pyridoxine hydrochloride	1401044-01	21678	60	20140221
Euro OTC	Pyridoxine hydrochloride	1407009-01	21773	60	20140807
Euro OTC	Pyridoxine hydrochloride	1507012	21846	60	20150721*
Euro OTC	Pyridoxine hydrochloride	1601039	22300	60	20160203*
Euro OTC	Pyridoxine hydrochloride	2211006	26439	40	20221125*
Fagron	Pyridoxine hydrochloride	22B07-B25-218396	26145	40	20220423

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 420 spectra of 8 reference samples from the substance/substance group *Pyridoxine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 542 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 540 spectra of 15 reference samples from the substance/substance group *Pyridoxine hydrochloride*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Pyridoxine hydrochloride	180287	24024	40
Caelo	Pyridoxine hydrochloride	21004047002	25973	40
Caelo	Pyridoxine hydrochloride	23001551	26839	40
Euro OTC	Pyridoxine hydrochloride	1604063	22569	40
Euro OTC	Pyridoxine hydrochloride	1608035	22798	40
Euro OTC	Pyridoxine hydrochloride	1710014	23735	40
Euro OTC	Pyridoxine hydrochloride	1806022-01	24189	40
Euro OTC	Pyridoxine hydrochloride	1908009	24838	40
Euro OTC	Pyridoxine hydrochloride	2107011	25778	50
Euro OTC	Pyridoxine hydrochloride	2204009	26227	40
Euro OTC	Pyridoxine hydrochloride	2309025	27001	40
Fagron	Pyridoxine hydrochloride	24A17-B09-236138	27171	40
Caelo	Pyridoxine hydrochloride	21004047002	25973SI	10
Euro OTC	Pyridoxine hydrochloride	2204009	26227SI	20
Fagron	Pyridoxine hydrochloride	22B07-B25-218396	26145SI†	20

- 201 544 spectra from a total of 4032 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

provided by the customer regarding manufacturer and batch number.

- 125 spectra from 35 *Apo-Ident* customers from 61 batches from the substance/substance group *Pyridoxine hydrochloride*.
- Among them are spectra of independent samples from 60 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Pyridoxine hydrochloride	21004047010	1
	Pyridoxine hydrochloride	24A17-B09-236138	1
Caelo	Pyridoxine hydrochloride	11021406	1
Caelo	Pyridoxine hydrochloride	11197009	1
Caelo	Pyridoxine hydrochloride	12102510	1
Caelo	Pyridoxine hydrochloride	12214102	2
Caelo	Pyridoxine hydrochloride	12214119	2
Caelo	Pyridoxine hydrochloride	13102509	2
Caelo	Pyridoxine hydrochloride	13102510	2
Caelo	Pyridoxine hydrochloride	13102516	1
Caelo	Pyridoxine hydrochloride	14262302	3
Caelo	Pyridoxine hydrochloride	14262306	1
Caelo	Pyridoxine hydrochloride	15218702	6
Caelo	Pyridoxine hydrochloride	15218707	1
Caelo	Pyridoxine hydrochloride	15218709	1
Caelo	Pyridoxine hydrochloride	15218710	2
Caelo	Pyridoxine hydrochloride	15218713	3
Caelo	Pyridoxine hydrochloride	16222501	5
Caelo	Pyridoxine hydrochloride	16222504	1
Caelo	Pyridoxine hydrochloride	16222506	2
Caelo	Pyridoxine hydrochloride	16222514	3
Caelo	Pyridoxine hydrochloride	16222515	2
Caelo	Pyridoxine hydrochloride	16222520	1
Caelo	Pyridoxine hydrochloride	16222521	1
Caelo	Pyridoxine hydrochloride	18028703	2
Caelo	Pyridoxine hydrochloride	18217603	1
Caelo	Pyridoxine hydrochloride	18217614	1
Caelo	Pyridoxine hydrochloride	19091203	2
Caelo	Pyridoxine hydrochloride	20003108002	2
Caelo	Pyridoxine hydrochloride	20003108003	1
Caelo	Pyridoxine hydrochloride	21004047002	1
Caesar & Loretz GmbH...	Pyridoxine hydrochloride	18217608	5
Caesar & Loretz GmbH...	Pyridoxine hydrochloride	11197009	5
Caesar & Loretz GmbH...	Pyridoxine hydrochloride	12214102	5
Caesar & Loretz GmbH...	Pyridoxine hydrochloride	12214110	2
Caesar & Loretz GmbH...	Pyridoxine hydrochloride	12214115	7
Caesar & Loretz GmbH...	Pyridoxine hydrochloride	12214119	2
Caesar & Loretz GmbH...	Pyridoxine hydrochloride	18217608	1
Caesar & Loretz GmbH...	Pyridoxine hydrochloride	19091203	1
Caesar & Loretz GmbH	Pyridoxine hydrochloride	18217603	1
Caesar & Loretz GmbH	Pyridoxine hydrochloride	18217606	1
Caesar & Loretz GmbH	Pyridoxine hydrochloride	190912002	2
Caesar & Loretz GmbH	Pyridoxine hydrochloride	19091203	1
Caesar & Loretz GmbH	Pyridoxine hydrochloride	19091204	1
Caesar & Loretz GmbH	Pyridoxine hydrochloride	21004047002	1
Euro OTC	Pyridoxine hydrochloride	1110001-01	1
Euro OTC	Pyridoxine hydrochloride	1206022-02	1
Euro OTC	Pyridoxine hydrochloride	1601039-01	1
Euro OTC	Pyridoxine hydrochloride	1604063-01	1
Euro OTC	Pyridoxine hydrochloride	160803501	1
Euro OTC	Pyridoxine hydrochloride	1608035-02	1
Euro OTC	Pyridoxine hydrochloride	17001401	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Pyridoxine hydrochloride	1710014-01	1
Euro OTC	Pyridoxine hydrochloride	1806022-01	1
Euro OTC	Pyridoxine hydrochloride	180602202	1
Euro OTC	Pyridoxine hydrochloride	1908009-02	5
Euro OTC	Pyridoxine hydrochloride	2204009-01	1
euro-oct	Pyridoxine hydrochloride	UQ60313085/0	1
Fagron	Pyridoxine hydrochloride	12e02-n02	1
Fagron	Pyridoxine hydrochloride	1608035-01	1
Fagron	Pyridoxine hydrochloride	20A29-F10-369782	1
Fagron	Pyridoxine hydrochloride	21A25-F01-376555	2
Fagron	Pyridoxine hydrochloride	21I01-B02-213683	1
Fagron	Pyridoxine hydrochloride	L13080030	1
Farmalabor	Pyridoxine hydrochloride	P1701531-000	1
Sanacorp	Pyridoxine hydrochloride	21004047008	2
Sanacorp	Pyridoxine hydrochloride	21004047010	2
Sanacorp	Pyridoxine hydrochloride	2211006-02	1
Sanacorp	Pyridoxine hydrochloride	23000263002	1
Sanacorp	Pyridoxine hydrochloride	23000263003	3

- 235 942 spectra from 1515 *Apo-Ident* customers from a total of 49 197 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Pyridoxine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Pyridoxine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	540	0	201 544
Type C	0	125	0	235 942

The substance/substance group *Pyridoxine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8889 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 95.2000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21675	21846	8.56	209.73
21678	21846	8.90	209.24
21773	21846	1.81	212.58
21846	21846	0.00	212.13
22300	22300	0.00	212.76
22770	22770	0.00	212.25
26145	21846	11.19	212.01
26439	26439	0.00	210.78

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Quetiapine fumarate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10005949-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Quetiapine fumarate; Quetiapini fumaras

Special notes

When selecting the *Quetiapine fumarate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Quetiapine fumarate	2	1	0

Second-stage model

For differentiation of the substance/substance group *Quetiapine fumarate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Quetiapine fumarate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	147.37	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Quetiapine fumarate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Quetiapine fumarate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Hetero Dru…	Quetiapine fumarate	QU22040055	26402	40	20220510
ZCL Chemic…	Quetiapine fumarate	QTP4206421	25834	50	2301088

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 90 spectra of 2 reference samples from the substance/substance group *Quetiapine fumarate*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

- 152 872 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 4 reference samples from the substance/substance group *Quetiapine fumarate*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
ZCL Chemicals Ltd.	Quetiapine fumarate	QTP4214921	25899	50
Hetero Drugs Ltd.	Quetiapine fumarate	QU22040055	26402SI†	20
ZCL Chemicals Ltd.	Quetiapine fumarate	QTP4206421	25834SI†	10
ZCL Chemicals Ltd.	Quetiapine fumarate	QTP4214921	25899SI	10

- 201 994 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Quetiapine fumarate*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Quetiapine fumarate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Quetiapine fumarate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	90	0	152 872
Type B	0	77	13	201 994
Type C	0	0	0	236 067

The substance/substance group *Quetiapine fumarate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 93.3333 %)
Type B	100.0000 % (> 99.9912 %)	85.5556 % (> 82.2222 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25834	25834	0.00	222.64
26402	25834	19.08	233.49

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Quinidine sulfate dihydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20819-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Quinidine sulfate dihydrate; Chinidini sulfas; Quinidine sulfate

Special notes

When selecting the *Quinidine sulfate dihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Quinidine sulfate dihydrate	6	4	5

Second-stage model

For differentiation of the substance/substance group *Quinidine sulfate dihydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Quinidine sulfate dihydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	91.17	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Quinidine sulfate dihydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Quinidine sulfate dihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Quinidine sulfate dihydrate	12L04-N10	20819	40	AR-14-FG-013249-01
Fagron	Quinidine sulfate dihydrate	12J16-B03	21217	39	1412323
Fagron	Quinidine sulfate dihydrate	14I04-B09-304357	21810	60	AR-15-FG-015409-01
Fagron	Quinidine sulfate dihydrate	22A17-B09-222135	26331	40	20220304
Fagron	Quinidine sulfate dihydrate	22A17-B09-222135	26331SI	20	20220304
Fagron	Quinidine sulfate dihydrate	23E17-B03-230370	26903	40	20230605
Fagron	Quinidine sulfate dihydrate	24E08-B13-001927	27408	40	20240705

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 279 spectra of 7 reference samples from the substance/substance group *Quinidine sulfate dihydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 683 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 6 reference samples from the substance/substance group *Quinidine sulfate dihydrate*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Quinidine sulfate dihydrate	16A06-B04-324954	22970	40
Fagron	Quinidine sulfate dihydrate	18B01-B08-350965	24181	40
Fagron	Quinidine sulfate dihydrate	20C23-F02-373172	25485	40
Fagron	Quinidine sulfate dihydrate	21E06-B01-213612	25901	40
Fagron	Quinidine sulfate dihydrate	21E06-B01-213612	25901SI	10
Fagron	Quinidine sulfate dihydrate	23E17-B03-230370	26903SI†	20

- 201 894 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5 spectra from 5 *Apo-Ident* customers from 5 batches from the substance/substance group *Quinidine sulfate dihydrate*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
buchler GmbH	Quinidine sulfate dihydrate	16a06-b04-340797	1
Caelo	Quinidine sulfate dihydrate	16A06-B04-330856	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Quinidine sulfate dihydrate	13G08-N02	1
Fagron	Quinidine sulfate dihydrate	18B01-B08-356315	1
Fagron	Quinidine sulfate dihydrate	21E06-B01-213612	1

- 236 062 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Quinidine sulfate dihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Quinidine sulfate dihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	279	0	152 683
Type B	0	190	0	201 894
Type C	0	5	0	236 062

The substance/substance group *Quinidine sulfate dihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8495 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20819	20819	0.00	191.09
21217	21217	0.00	191.36
21810	21810	0.00	190.89

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26331	21810	9.50	191.38
26903	21810	4.35	193.39
27408	21810	8.86	191.22

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Quinine hydrochloride dihydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20547-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Quinine hydrochloride dihydrate; Chinini hydrochloridum dihydricum

Special notes

When selecting the *Quinine hydrochloride dihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Quinine hydrochloride dihydrate	7	3	15

Second-stage model

For differentiation of the substance/substance group *Quinine hydrochloride dihydrate* the following second-stage model is used:

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Quinine hydrochloride dihydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	84.47	–
⋮	⋮	⋮
Capsaicin	>50	160.26
Ciprofloxacin hydrochloride	>50	164.22
Sodium citrate	>50	167.15
Oxybutynin hydrochloride	>50	194.60
Levocarnitine	>50	289.61
Heparin sodium	>50	299.85
Pyridoxal-5-phosphate	>50	311.98
Methoxsalen	>50	362.34
Prednicarbate	>50	379.50
Cyproterone acetate	>50	471.39
Tetracaine	>50	519.15
Triclosan	>50	596.22
Alfatradiol	>50	663.84
Sucrose	>50	894.45
Norethisterone acetate	>50	1017.89
Amitriptyline hydrochloride	>50	1120.69
Amifampridine	>50	1150.67
Valine	>50	1652.84

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Quinine hydrochloride dihydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Quinine hydrochloride dihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Quinine hydrochloride dih…	15376201	22309	60	20151105
Caelo	Quinine hydrochloride dih…	16283302	23577	40	1802260

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Quinine hydrochloride dih…	20002720	25621	40	20201119*
Fagron	Quinine hydrochloride dih…	13G10-N07	21235	30	20130809
Fagron	Quinine hydrochloride dih…	13I30-B02-295630	21809	60	AR-15-FG-015410-01
Fagron	Quinine hydrochloride dih…	20B26-F03-370029	25491	40	20200501
Fagron	Quinine hydrochloride dih…	21E06-B02-213598	26332	40	20210615
Fagron	Quinine hydrochloride dih…	21E06-B02-213598	26332SI	20	20210615

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 330 spectra of 8 reference samples from the substance/substance group *Quinine hydrochloride dihydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 632 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Quinine hydrochloride dihydrate*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Quinine hydrochloride dih…	180226	24022	40
Fagron	Quinine hydrochloride dih…	15A20-B03-319027	23573	40
Fagron	Quinine hydrochloride dih…	16K01-B05-340171	23920	40

- 201 964 spectra from a total of 4042 batches from further 838 substances. These spectra were

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 24 spectra from 20 *Apo-Ident* customers from 18 batches from the substance/substance group *Quinine hydrochloride dihydrate*.
- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Quinine hydrochloride dih…	12316604	1
Caelo	Quinine hydrochloride dih…	12316605	1
Caelo	Quinine hydrochloride dih…	12316611	2
Caelo	Quinine hydrochloride dih…	12316617	1
Caelo	Quinine hydrochloride dih…	13D24-N06	1
Caelo	Quinine hydrochloride dih…	15227701	1
Caelo	Quinine hydrochloride dih…	15376201	2
Caelo	Quinine hydrochloride dih…	153776201	1
Caelo	Quinine hydrochloride dih…	153796204	1
Caelo	Quinine hydrochloride dih…	16283302	1
Caelo	Quinine hydrochloride dih…	16283305	3
Caelo	Quinine hydrochloride dih…	180226002	1
Caelo	Quinine hydrochloride dih…	18022602	1
Caelo	Quinine hydrochloride dih…	18022604	1
Caelo	Quinine hydrochloride dih…	18022605	1
Caesar & Loretz GmbH	Quinine hydrochloride dih…	180226002	1
Caesar & Loretz GmbH	Quinine hydrochloride dih…	18022605	1
Fagron	Quinine hydrochloride dih…	10N129B	1
Fagron	Quinine hydrochloride dih…	13G10-N07	1
Gatt-Koller	Quinine hydrochloride dih…	3500/08103810	1

- 236 043 spectra from 1515 *Apo-Ident* customers from a total of 49 240 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Quinine hydrochloride dihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Quinine hydrochloride dihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	330	0	152 632
Type B	0	120	0	201 964
Type C	0	24	0	236 043

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The substance/substance group *Quinine hydrochloride dihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1818 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 75.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21235	25621	16.92	188.97
21809	21809	0.00	147.34
22309	23577	6.02	161.99
23577	23577	0.00	164.17
25491	23577	10.02	178.61
25621	25621	0.00	184.54
26332	21809	10.02	155.23

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Quinine sulfate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21057-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Quinine sulfate; Chinini sulfas

Special notes

When selecting the *Quinine sulfate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Quinine sulfate	6	2	6

Second-stage model

For differentiation of the substance/substance group *Quinine sulfate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Quinine sulfate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	101.73	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Quinine sulfate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Quinine sulfate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Quinine sulfate	13024604	21429	60	AR-16-FG-005472-01
Caelo	Quinine sulfate	15230005	22959	40	20150729
Fagron	Quinine sulfate	13J23-N03	21057	40	1404401
Fagron	Quinine sulfate	14B27-B01	21277	40	AR-16-FG-009455-01
Fagron	Quinine sulfate	22B24-B03-216222	26143	40	20220423
Fagron	Quinine sulfate	22B24-B03-216222	26143SI	20	20220423
Fagron	Quinine sulfate	23C09-B03-229466	26681	40	20230327
Fagron	Quinine sulfate	23C09-B03-229466	26681SI	20	20230327

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 300 spectra of 8 reference samples from the substance/substance group *Quinine sulfate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 662 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Quinine sulfate*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Quinine sulfate	170616	23281	40
Caelo	Quinine sulfate	180630	24032	40
Caelo	Quinine sulfate	170616	23316	40

- 201 964 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 9 spectra from 3 *Apo-Ident* customers from 6 batches from the substance/substance group *Quinine sulfate*.
- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Quinine sulfate	15B06B03304359	1
Gatt-Koller / Phoenix	Quinine sulfate	2503/07143314	1
Gatt-Koller / Phoenix	Quinine sulfate	4928/11132214	1
Gatt-Koller	Quinine sulfate	1801042	1
Gatt-Koller	Quinine sulfate	1803149	4
KÖGL	Quinine sulfate	1901102	1

- 236 058 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further

721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Quinine sulfate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Quinine sulfate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	120	0	201 964
Type C	0	8	1	236 058

The substance/substance group *Quinine sulfate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21057	21057	0.00	177.65
21277	21277	0.00	173.40
21429	21429	0.00	177.23
22959	21429	9.69	173.27
26143	21277	7.39	167.57
26681	21057	10.48	171.51

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Quinoline yellow**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20456-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Quinoline yellow

Special notes

When selecting the *Quinoline yellow* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Quinoline yellow	6	3	57

Second-stage model

For differentiation of the substance/substance group *Quinoline yellow* the following second-stage model is used:

- Submodel 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Quinoline yellow* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	61.11	–
⋮	⋮	⋮
Saccharin sodium	>50	25.96
Atropine sulfate	>50	107.25
Mometasone furoate	>50	110.07
Escin, water-soluble	>50	122.51
Magnesium hydrogen citrate	>50	189.44
Propranolol hydrochloride	>50	212.25
Hydrocortisone	>50	251.29
Phenytoin	>50	375.31
Potassium sorbate	>50	383.54
Calcium orotate dihydrate	>50	434.29

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Quinoline yellow* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Quinoline yellow*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Quinoline yellow	12042010	20922	40	20120314
Caelo	Quinoline yellow	13109108	21305	40	1711481
Caelo	Quinoline yellow	17034101	23400	40	1709327
Caelo	Quinoline yellow	172277	23685	30	20171020*
Caelo	Quinoline yellow	172277	24812	40	20171020*
Caelo	Quinoline yellow	20002519012	26737	40	231105522
Caelo	Quinoline yellow	23002618	26962	40	20231103*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 270 spectra of 7 reference samples from the substance/substance group *Quinoline yellow*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 692 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 220 spectra of 6 reference samples from the substance/substance group *Quinoline yellow*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Quinoline yellow	16050101	23401	40
Caelo	Quinoline yellow	190734	24555	40
Fagron	Quinoline yellow	12E24-N01	20731	60
Caelo	Quinoline yellow	190734	24725	40
Caelo	Quinoline yellow	20002519012	26737SI†	20
Caelo	Quinoline yellow	23002618	26962SI†	20

- 201 864 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 179 spectra from 99 *Apo-Ident* customers from 60 batches from the substance/substance group *Quinoline yellow*.

- Among them are spectra of independent samples from 57 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Quinoline yellow	20002519008	1
	Quinoline yellow	20002519011	1
Caelo	Quinoline yellow	11089606	1
Caelo	Quinoline yellow	11089608	1
Caelo	Quinoline yellow	11089610	1
Caelo	Quinoline yellow	118E-03146	1
Caelo	Quinoline yellow	12042002	3
Caelo	Quinoline yellow	12042004	1
Caelo	Quinoline yellow	12042007	3
Caelo	Quinoline yellow	12042010	1
Caelo	Quinoline yellow	12051810	1
Caelo	Quinoline yellow	13109102	2
Caelo	Quinoline yellow	13109109	1
Caelo	Quinoline yellow	14049401	2
Caelo	Quinoline yellow	14274305	1
Caelo	Quinoline yellow	14274309	1
Caelo	Quinoline yellow	14363202	4
Caelo	Quinoline yellow	14363207	1
Caelo	Quinoline yellow	15276801	2
Caelo	Quinoline yellow	15276802	1
Caelo	Quinoline yellow	15276803	2
Caelo	Quinoline yellow	15276804	2
Caelo	Quinoline yellow	16050101	8
Caelo	Quinoline yellow	16050106	4
Caelo	Quinoline yellow	16050108	2
Caelo	Quinoline yellow	17034101	4
Caelo	Quinoline yellow	17034102	7
Caelo	Quinoline yellow	17034104	7
Caelo	Quinoline yellow	172277003	1
Caelo	Quinoline yellow	17227701	9
Caelo	Quinoline yellow	17227702	1
Caelo	Quinoline yellow	17227703	7
Caelo	Quinoline yellow	17227705	1
Caelo	Quinoline yellow	17227706	9
Caelo	Quinoline yellow	17227708	1
Caelo	Quinoline yellow	17227709	4
Caelo	Quinoline yellow	190734001	1
Caelo	Quinoline yellow	190734002	5
Caelo	Quinoline yellow	190734003	10
Caelo	Quinoline yellow	190734004	4
Caelo	Quinoline yellow	19073401	12
Caelo	Quinoline yellow	20002519003	1
Caelo	Quinoline yellow	20002519004	1
Caelo	Quinoline yellow	20002519005	3
Caelo	Quinoline yellow	20002519006	2
Caelo	Quinoline yellow	20301211-6	1
Caelo	Quinoline yellow	713E-03146	1
Caesar & Loretz GmbH...	Quinoline yellow	20002519012	1
Caesar & Loretz GmbH...	Quinoline yellow	20002519003	1
Caesar & Loretz GmbH	Quinoline yellow	17227705	1
Caesar & Loretz GmbH	Quinoline yellow	190734001	4
Caesar & Loretz GmbH	Quinoline yellow	190734002	1
Caesar & Loretz GmbH	Quinoline yellow	190734003	1
Caesar & Loretz GmbH	Quinoline yellow	190734004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Quinoline yellow	19073401	2
Caesar & Loretz GmbH	Quinoline yellow	20002519003	1
Caesar & Loretz GmbH	Quinoline yellow	20002519004	2
Caesar & Loretz GmbH	Quinoline yellow	20002519005	2
Caesar & Loretz GmbH	Quinoline yellow	20002519007	1
Caesar & Loretz GmbH	Quinoline yellow	20002519008	2
Caesar & Loretz GmbH	Quinoline yellow	20002519009	1
Caesar & Loretz GmbH	Quinoline yellow	2002519006	1
Fagron	Quinoline yellow	100427	1
Fagron	Quinoline yellow	11F30-N04	1
Fagron	Quinoline yellow	11K08-N01	2
Fagron	Quinoline yellow	12B08-N08	1
Fagron	Quinoline yellow	12E24-N05	1
Fagron	Quinoline yellow	12L11-N07	1
Fagron	Quinoline yellow	14D18-B02-295783	1
Fagron	Quinoline yellow	17227705	1
Fagron	Quinoline yellow	9878	1
Klosterring	Quinoline yellow	17227706	1
Noweda	Quinoline yellow	17227706	1
PHOENIX	Quinoline yellow	12042004	1
Phoenix	Quinoline yellow	20002519003	1
phönix	Quinoline yellow	15276803	1
Phönix	Quinoline yellow	16050108	1
sanacorp	Quinoline yellow	3214M-03146	1

- 235 888 spectra from 1515 *Apo-Ident* customers from a total of 49 198 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Quinoline yellow* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Quinoline yellow* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	270	0	152 692
Type B	0	220	0	201 864
Type C	0	179	0	235 888

The substance/substance group *Quinoline yellow* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7778 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.2727 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 96.6480 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20922	21305	17.46	141.55
21305	21305	0.00	136.85
23400	23400	0.00	149.31
23685	23685	0.00	145.31
24812	24812	0.00	138.66
26737	26737	0.00	129.23
26962	26962	0.00	147.42

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Resocrinol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20938-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Resocrinol; Resorcinolum

Special notes

When selecting the *Resocrinol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Resocrinol	9	5	102

Second-stage model

For differentiation of the substance/substance group *Resocrinol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Resocrinol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Hydroquinone	37.32	–
Sodium cromoglicate	97.96	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Resocrinol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Resocrinol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Resocrinol	13293108	21471	60	AR-15-FG-006906-01
Caelo	Resocrinol	161533	22632	40	20160524*
Caelo	Resocrinol	182166	25196	40	20181114*
Caelo	Resocrinol	22002981	26504	40	20221014*
Caelo	Resocrinol	22002981	26504SI	20	20221014*
Caelo	Resocrinol	23001796	26969	40	20230814*
Caelo	Resocrinol	23001796	26969SI	20	20230814*
Caelo	Resocrinol	24000513	27136	40	20240226*
Fagron	Resocrinol	12G24-N04	20938	40	1401462
Fagron	Resocrinol	13I18-B09-291533	21706	40	20130606
Fagron	Resocrinol	19J21-B16-195450	25171	40	20191105

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 420 spectra of 11 reference samples from the substance/substance group *Resocrinol*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 542 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 225 spectra of 7 reference samples from the substance/substance group *Resocrinol*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Resocrinol	20003735	25736	50
Caelo	Resocrinol	21004158	26005	40
Caelo	Resocrinol	23003284	27117	40
Fagron	Resocrinol	17H03-B11-338899	23921	40
Fagron	Resocrinol	21F14-B01-213197	27240	40
Caelo	Resocrinol	21004158	26005SI	10
Fagron	Resocrinol	13I18-B09-291533	21706†	5

- 201 859 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 246 spectra from 167 *Apo-Ident* customers from 108 batches from the substance/substance group *Resocrinol*.

- Among them are spectra of independent samples from 102 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Resocrinol	21004158004	1
	Resocrinol	21004158008	2
	Resocrinol	21F14-B01-213197	1
	Resocrinol	22002981004	2
	Resocrinol	90972	1
Anzag	Resocrinol	18216615	1
Caelo	Resocrinol	10111210	1
Caelo	Resocrinol	10218809	2
Caelo	Resocrinol	11309610	4
Caelo	Resocrinol	11d29-n14	2
Caelo	Resocrinol	12255614	2
Caelo	Resocrinol	12G24-N04	2
Caelo	Resocrinol	13/18-B19-291534	1
Caelo	Resocrinol	13293103	1
Caelo	Resocrinol	13293110	1
Caelo	Resocrinol	13293115	2
Caelo	Resocrinol	15009502	1
Caelo	Resocrinol	15009507	8
Caelo	Resocrinol	15009511	4
Caelo	Resocrinol	15009515	2
Caelo	Resocrinol	15K24-B02-317584	1
Caelo	Resocrinol	16/13082	1
Caelo	Resocrinol	16153306	1
Caelo	Resocrinol	16153307	1
Caelo	Resocrinol	16153309	8
Caelo	Resocrinol	16153312	1
Caelo	Resocrinol	16153313	5
Caelo	Resocrinol	16271807	1
Caelo	Resocrinol	16D29-B01	1
Caelo	Resocrinol	18015601	1
Caelo	Resocrinol	18015603	1
Caelo	Resocrinol	18111703	1
Caelo	Resocrinol	18130901	3
Caelo	Resocrinol	182166002	1
Caelo	Resocrinol	18216601	1
Caelo	Resocrinol	18216603	7
Caelo	Resocrinol	18216607	2
Caelo	Resocrinol	18216609	1
Caelo	Resocrinol	18216610	1
Caelo	Resocrinol	18216611	7
Caelo	Resocrinol	18216615	1
Caelo	Resocrinol	18B08-B05-347787	3
Caelo	Resocrinol	19061305	1
Caelo	Resocrinol	19J21-16-I95450	1
Caelo	Resocrinol	20003735002	2
Caelo	Resocrinol	20003735007	3
Caelo	Resocrinol	2003735006	1
Caelo	Resocrinol	2041512	1
Caelo	Resocrinol	206370-0003	1
Caelo	Resocrinol	21004158004	2
Caelo	Resocrinol	24092001	1
Caelo	Resocrinol	5052	1
Caesar & Loretz GmbH...	Resocrinol	18216603	1
Caesar & Loretz GmbH/Gehe	Resocrinol	182166002	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/L30	Resocrinol	21000873008	1
Caesar & Loretz GmbH...	Resocrinol	20003735007	1
Caesar & Loretz GmbH...	Resocrinol	18216601	1
Caesar & Loretz GmbH	Resocrinol	18216607	1
Caesar & Loretz GmbH	Resocrinol	18216609	1
Caesar & Loretz GmbH	Resocrinol	18216611	1
Caesar & Loretz GmbH	Resocrinol	18216613	1
Caesar & Loretz GmbH	Resocrinol	20003735005	2
Caesar & Loretz GmbH	Resocrinol	20003735006	2
Caesar & Loretz GmbH	Resocrinol	20003735007	1
Euro OTC	Resocrinol	11/13-N02	1
Euro OTC	Resocrinol	16D29-B01-329760	1
Fagron	Resocrinol	10B01-N06	2
Fagron	Resocrinol	11/13-N02	2
Fagron	Resocrinol	11/13-no2	1
Fagron	Resocrinol	1112013A	1
Fagron	Resocrinol	118b09291534	1
Fagron	Resocrinol	11A19-N09	1
Fagron	Resocrinol	11D29-N14	1
Fagron	Resocrinol	11L19-N19	2
Fagron	Resocrinol	12G24-N004	1
Fagron	Resocrinol	12g24-N04	1
Fagron	Resocrinol	12G24-N04	9
Fagron	Resocrinol	12K30-N03	4
Fagron	Resocrinol	13/17071	1
Fagron	Resocrinol	13/18-B09-291534	1
Fagron	Resocrinol	13E24-N10	8
Fagron	Resocrinol	13I18-B09	2
Fagron	Resocrinol	13I18-B09-291533	1
Fagron	Resocrinol	13I18-B09-291534	1
Fagron	Resocrinol	14/15-B02-307749	1
Fagron	Resocrinol	14/16062	1
Fagron	Resocrinol	14/19050	1
Fagron	Resocrinol	1415B02307749	1
Fagron	Resocrinol	14G10B06	1
Fagron	Resocrinol	14G10-B06-296296	7
Fagron	Resocrinol	14G10-B06-296297	2
Fagron	Resocrinol	14J15-B02	2
Fagron	Resocrinol	14J15-B02-307749	5
Fagron	Resocrinol	15/18082	1
Fagron	Resocrinol	15K24-B02-317584	3
Fagron	Resocrinol	1613082	1
Fagron	Resocrinol	16D29-B01	1
Fagron	Resocrinol	16d29b01323046	1
Fagron	Resocrinol	16D29-B01-323046	5
Fagron	Resocrinol	16D29-B01-329760	3
Fagron	Resocrinol	16d29b01332738	1
Fagron	Resocrinol	16D29-B01-332738	2
Fagron	Resocrinol	17H03-B11-338899	3
Fagron	Resocrinol	17H03-B11-342399	1
Fagron	Resocrinol	18/19081	1
Fagron	Resocrinol	18B08-B05-347787	5
Fagron	Resocrinol	18K20-B01-355679	1
Fagron	Resocrinol	19J21-B16195450	1
Fagron	Resocrinol	19J21-B16-195450	1
Fagron	Resocrinol	20E07-B09-200551	2
Fagron	Resocrinol	20129-B13	1
Fagron	Resocrinol	20L29-B13	2
Fagron	Resocrinol	20L29-B13-204180	6
Fagron	Resocrinol	211217(20L29-B13-204180)	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Resocrinol	2112I-02170	1
Fagron	Resocrinol	88735	1
Fagron	Resocrinol	B09-2005501	1
Fagron	Resocrinol	B16-1954500	1
Fargon/ Phönix	Resocrinol	16D29-B01-323046	1
Fargon	Resocrinol	15K24-B02-317584	1
Gehe	Resocrinol	11L13-N02	1
Gehe	Resocrinol	13E24-N10	1
L12	Resocrinol	16153306	1
Noweda/Fargon	Resocrinol	16029-B01-329760	1
Noweda	Resocrinol	1318b09291533	1
Noweda	Resocrinol	13E24-N10	1
Noweda	Resocrinol	14G10-B06-296	1
Noweda	Resocrinol	2003735007	1
Noweda	Resocrinol	21004158004	1
Phoenix WE: 13.07.2015	Resocrinol	14G10-B06-296296	1
Phoenix goettin	Resocrinol	13I18-B09-291534	1
Phönix Gotha	Resocrinol	14G10-B06-296296	1
Phönix	Resocrinol	20L29-B13	1
Sanacorp	Resocrinol	16D29-Bo1-323046	1
vdl	Resocrinol	12G24-N04	1

- 235 821 spectra from 1515 *Apo-Ident* customers from a total of 49 151 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Resocrinol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Resocrinol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	225	0	201 859
Type C	0	245	1	235 821

The substance/substance group *Resocrinol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.3333 %)
Type C	100.0000 % (> 99.9007 %)	99.5935 % (> 98.3740 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20938	20938	0.00	49.80
21471	21471	0.00	45.15
21706	21471	7.64	41.09
22632	22632	0.00	44.61
25171	21471	11.27	40.74
25196	25196	0.00	43.77
26504	26504	0.00	41.39
26969	26969	0.00	56.15
27136	27136	0.00	44.97

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Riboflavin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20409-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Riboflavin; Riboflavinum

Special notes

When selecting the *Riboflavin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Riboflavin	12	13	64

Second-stage model

For differentiation of the substance/substance group *Riboflavin* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Riboflavin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	32.70	11.00
Riboflavin sodium phosphate hydrate	32.95	–
Sodium cromoglicate	69.24	–
⋮	⋮	⋮
Bacitracin	>50	30.58
Colistin sulfate	>50	31.64
Amphotericin B	>50	44.66
Cyanocobalamin	>50	55.10
Calcium pantothenate	>50	57.25
Nystatin	>50	57.71
Triamcinolone	>50	62.49
Tosylchloramide sodium	>50	64.32
Calcium glycerophosphate	>50	76.30
Estradiol hemihydrate	>50	76.82
Hyoscine hydrobromide	>50	79.63
alpha-tocopheryl acetate dry concentrate	>50	100.70
SyrSpend® SF pH4 neo (Maize starch)	>50	101.74
Selenium yeast	>50	104.42
Estriol	>50	115.13
Methylcobalamin	>50	118.32
Gelatine, white	>50	124.32
Carmellose sodium	>50	156.01
SyrSpend® SF Alka	>50	157.36
Rice starch	>50	164.48
Oxalic acid	>50	198.69
SyrSpend® SF pH4	>50	252.66
Corn starch	>50	268.93
Wheat starch	>50	282.41
Acacia, dried dispersion	>50	307.30
Potato starch	>50	312.39
Fructose	>50	318.91
Maltodextrin	>50	350.99

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Riboflavin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Riboflavin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Riboflavin	12003317	20925	40	1405155
Caelo	Riboflavin	13305203	21389	60	AR-15-FG-005686-01
Caelo	Riboflavin	14322008	22492	40	AR-16-FG-013669-01
Caelo	Riboflavin	21000916	25654	40	20210408*
Euro OTC	Riboflavin	1701050	23004	40	20170214*
Euro OTC	Riboflavin	1701050-01	23091	40	20170214
Euro OTC	Riboflavin	2002026	25157	40	20200512*
Euro OTC	Riboflavin	2102005	25600	40	20210330*
Fagron	Riboflavin	13D02-N03	20825	40	AR-15-FG-000733-01
Fagron	Riboflavin	13D02-N03	20914	40	20130405
Fagron	Riboflavin	15G20-B13-310997	21955	60	20150819
Fagron	Riboflavin	16B18-B06-319026	22655	40	AR-16-FG-014466-01
Fagron	Riboflavin	17G14-B05-337885	23714	40	AR-18-FG-000141-01

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 560 spectra of 13 reference samples from the substance/substance group *Riboflavin*. These samples are listed above in the *calibration samples* section. The reference samples come from 12 different batches.
- 152 402 spectra from a total of 2830 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 600 spectra of 17 reference samples from the substance/substance group *Riboflavin*.
- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Riboflavin	15330708	23579	40
Caelo	Riboflavin	172722	23649	40
Caelo	Riboflavin	192609	24884	40
Caelo	Riboflavin	22003300	26473	40
Caelo	Riboflavin	23003154	27129	40
Euro OTC	Riboflavin	1707017	23612	40
Euro OTC	Riboflavin	1801018	23880	40
Euro OTC	Riboflavin	1809004	24297	40
Euro OTC	Riboflavin	1810005	24307	40
Euro OTC	Riboflavin	2009015	25423	40
Euro OTC	Riboflavin	2210022	26437	40
Euro OTC	Riboflavin	2408013	27401	40
Fagron	Riboflavin	22D13-B02-219504	26398	40
Caelo	Riboflavin	22003300	26473SI	20
Caelo	Riboflavin	23003154	27129SI	20
Euro OTC	Riboflavin	2408013	27401SI	20
Fagron	Riboflavin	22D13-B02-219504	26398SI	20

- 201 484 spectra from a total of 4032 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 111 spectra from 47 *Apo-Ident* customers from 69 batches from the substance/substance group *Riboflavin*.

- Among them are spectra of independent samples from 64 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Riboflavin	20004481001	1
	Riboflavin	22003300001	1
Anzag/Anzag 11.09.18	Riboflavin	18B22-B01-347142	1
Caelo	Riboflavin	15330708	2
Caelo	Riboflavin	17272204	2
Caelo	Riboflavin	17G14-B05-337885	1
Caelo	Riboflavin	21000916002	2
Caelo	Riboflavin	21000916003	1
Caelo	Riboflavin	21000916007	1
Caesar & Loretz GmbH...	Riboflavin	19000560002	1
Caesar & Loretz GmbH...	Riboflavin	18123401	1
Caesar & Loretz GmbH	Riboflavin	19000560002	1
Caesar & Loretz GmbH	Riboflavin	21000916002	1
EuRho	Riboflavin	1810005-01	1
Euro OTC	Riboflavin	1701050-02	1
Euro OTC	Riboflavin	1707017-01	1
Euro OTC	Riboflavin	19G17-B07	1
Euro OTC	Riboflavin	2102005-02	1
Euro OTC	Riboflavin	L1210048-01	1
Euro OTC	Riboflavin	L1305039-01	1
Fagr9n 06.11.19	Riboflavin	19F10B07191754	1
Fagron	Riboflavin	11K02-N01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Riboflavin	13J29-B04-287533	1
Fagron	Riboflavin	13J29-B04-287534	1
Fagron	Riboflavin	14B03B07292071	1
Fagron	Riboflavin	14E01-B10-296718	2
Fagron	Riboflavin	14K03-B04-304718	1
Fagron	Riboflavin	15G20-B13-310997	2
Fagron	Riboflavin	15I09-B02-315216	1
Fagron	Riboflavin	167720-0005	2
Fagron	Riboflavin	16B18_b06_319026	1
Fagron	Riboflavin	16B18-B06-321484	1
Fagron	Riboflavin	16E18-B05-325274	1
Fagron	Riboflavin	16E-18-B05-325274	1
Fagron	Riboflavin	16I12-B05-329618	1
Fagron	Riboflavin	16J12-B05-329618	2
Fagron	Riboflavin	1701050-01	1
Fagron	Riboflavin	17G14-B05-337885	1
Fagron	Riboflavin	17H10-B06-340170	3
Fagron	Riboflavin	18822-B01-347142	2
Fagron	Riboflavin	18D05-B04	1
Fagron	Riboflavin	18D05B04349962	1
Fagron	Riboflavin	18J10-B01	2
Fagron	Riboflavin	18J10-B01-355004	4
Fagron	Riboflavin	18J10-B01-356142	1
Fagron	Riboflavin	19F10-B07-191754	4
Fagron	Riboflavin	19F-10-B07-191754	1
Fagron	Riboflavin	19g17-b07-192788	1
Fagron	Riboflavin	19G17-B07-192788	5
Fagron	Riboflavin	19G17-B07-200577	5
Fagron	Riboflavin	19GT-B07-192788	2
Fagron	Riboflavin	20a14-b04-196790	1
Fagron	Riboflavin	20A14-B04-196790	1
Fagron	Riboflavin	20A14-BO4-196790	1
Fagron	Riboflavin	21A14-B03-210578	6
Fagron	Riboflavin	21D07-B10-218559	3
Fagron	Riboflavin	22B26-B01	1
Fagron	Riboflavin	22D13-B02	3
Fagron	Riboflavin	22D13-B02-219504	3
Fagron	Riboflavin	22L13-B16-226589	1
Fagron	Riboflavin	B04-1967900	1
Fagron	Riboflavin	BO4-1967900	1
Fagron	Riboflavin	BO7-2005707	1
Fagron	Riboflavin	RIB3061HF	2
Fagron	Riboflavin	UQ00510683	1
Fagron	Riboflavin	UQ60910194	1
Fagron	Riboflavin	UQ70210050	1
Fagron	Riboflavin	UQ80810145	1
Fagron	Riboflavin	UQ90410074	1
Gatt-Koller	Riboflavin	1803007	1
Noweda	Riboflavin	18J10-B01-355004	1
Noweda	Riboflavin	19F01-B07-191754	1
Vdl 09.05.14;Preis 7,45	Riboflavin	13305203/15R05	1

- 235 956 spectra from 1515 *Apo-Ident* customers from a total of 49 189 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Riboflavin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Riboflavin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	560	0	152 402
Type B	0	600	0	201 484
Type C	0	110	1	235 956

The substance/substance group *Riboflavin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9286 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0000 %)
Type C	100.0000 % (> 99.9007 %)	99.0991 % (> 96.3964 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20825	20825	0.00	85.48
20914	20825	15.04	85.53
20925	20925	0.00	92.48
21389	21389	0.00	93.13
21955	21389	12.70	96.06
22492	22492	0.00	101.26
22655	22655	0.00	98.91
23004	23004	0.00	90.90
23091	23714	19.20	93.75
23714	23714	0.00	96.81
25157	25157	0.00	91.43
25600	25600	0.00	111.95
25654	25654	0.00	101.63

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Riboflavin sodium phosphate hydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20948-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Riboflavin sodium phosphate hydrate; Riboflavini natrii phosphas hydricum

Special notes

When selecting the *Riboflavin sodium phosphate hydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Riboflavin sodium phosphate hydrate	8	3	3

Second-stage model

For differentiation of the substance/substance group *Riboflavin sodium phosphate hydrate* the following second-stage model is used:

- Submodel 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Riboflavin sodium phosphate hydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	40.36	–
Carbomers	41.52	41.89
Magnesium citrate	47.70	34.91
⋮	⋮	⋮
Mg-Ca-K colamine phosphate	>50	109.18
Gentamicin sulfate	>50	112.26
Neomycin sulfate	>50	223.58
Tobramycin sulfate	>50	283.06
Zinc gluconate	>50	344.56
Sodium tetraborate	>50	650.64
Finasteride	>50	747.82

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Riboflavin sodium phosphate hydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Riboflavin sodium phosphate hydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Riboflavin sodium phospha…	2306014	26856	40	20230831*
Fagron	Riboflavin sodium phospha…	13I26-N06	20948	40	1403705
Fagron	Riboflavin sodium phospha…	15J02-B03-313137	22269	60	AR-16-FG-009883-02
Fagron	Riboflavin sodium phospha…	17A03-B01-335897	23713	40	AR-18-FG-000920-01
Fagron	Riboflavin sodium phospha…	20L02-B02-202655	25494	40	2105284
Fagron	Riboflavin sodium phospha…	21E19-B01-213684	26162	40	20210702
Fagron	Riboflavin sodium phospha…	22D20-B02-221099	26461	40	20220625
Fagron	Riboflavin sodium phospha…	23E16-B05-229478	26829	40	20230602
Fagron	Riboflavin sodium phospha…	23E16-B05-229478	26829SI	20	20230602

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Riboflavin sodium phosphate hydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 602 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 165 spectra of 5 reference samples from the substance/substance group *Riboflavin sodium phosphate hydrate*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Riboflavin sodium phospha…	2302008	26659	40
Fagron	Riboflavin sodium phospha…	14J31-B07-300519	21707	45
Fagron	Riboflavin sodium phospha…	17H03-B13-347175	24113	40
Euro OTC	Riboflavin sodium phospha…	2302008	26659SI	20
Fagron	Riboflavin sodium phospha…	21E19-B01-213684	26162SI†	20

- 201 919 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 6 spectra from 1 *Apo-Ident* customers from 5 batches from the substance/substance group *Riboflavin sodium phosphate hydrate*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Fagron	Riboflavin sodium phospha…	20H27	1
Fagron	Riboflavin sodium phospha…	20H27-B07-201994	1
Fagron	Riboflavin sodium phospha…	20L02-B02-202655	1
Fagron	Riboflavin sodium phospha…	21E19-B01-213684	2
Sigma Aldrich	Riboflavin sodium phospha…	MKCG3538	1

- 236 061 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Riboflavin sodium phosphate hydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Riboflavin sodium phosphate hydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	165	0	201 919
Type C	0	6	0	236 061

The substance/substance group *Riboflavin sodium phosphate hydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.3636 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20948	20948	0.00	52.83
22269	22269	0.00	66.92
23713	23713	0.00	93.03
25494	25494	0.00	98.78
26162	25494	17.70	113.23
26461	25494	9.76	102.30
26829	25494	47.32	129.02
26856	26856	0.00	82.38

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ropivacaine hydrochloride monohydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10002307-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ropivacaine hydrochloride monohydrate; Ropivacaini hydrochloridum monohydricum

Special notes

When selecting the *Ropivacaine hydrochloride monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ropivacaine hydrochloride monohydrate	5	2	0

Second-stage model

For differentiation of the substance/substance group *Ropivacaine hydrochloride monohydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ropivacaine hydrochloride monohydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prednisolon dihydrogen phosphate di…	78.07	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ropivacaine hydrochloride monohydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ropivacaine hydrochloride monohydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ropivacaine hydrochloride…	181569	24871	40	20180802*
Euro OTC	Ropivacaine hydrochloride…	1707006	23704	40	20171013*
Euro OTC	Ropivacaine hydrochloride…	1903027	24607	40	20190416*
Fagron	Ropivacaine hydrochloride…	20I17-F09-375251	25920	40	2204443
Fagron	Ropivacaine hydrochloride…	22D25-B06	26444	40	20220812*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Ropivacaine hydrochloride monohydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 762 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 3 reference samples from the substance/substance group *Ropivacaine hydrochloride monohydrate*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ropivacaine hydrochloride…	191139	24872	40
Euro OTC	Ropivacaine hydrochloride…	2106016	25919	40
Euro OTC	Ropivacaine hydrochloride…	2106016	25919SI	10

- 201 994 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Ropivacaine hydrochloride monohydrate*.

- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ropivacaine hydrochloride monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*.

For this purpose, all relevant spectra of the various substances were compared with *Ropivacaine hydrochloride monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	90	0	201 994
Type C	0	0	0	236 067

The substance/substance group *Ropivacaine hydrochloride monohydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 93.3333 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23704	23704	0.00	185.52
24607	24607	0.00	181.65
24871	24871	0.00	177.25
25920	25920	0.00	169.94
26444	26444	0.00	178.38

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Saccharin sodium**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20200-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Saccharin sodium; Saccharinum natricum; Sodium saccharin

Special notes

When selecting the *Saccharin sodium* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Saccharin sodium	10	6	76

Second-stage model

For differentiation of the substance/substance group *Saccharin sodium* the following second-stage model is used:

- Submodel 14

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Saccharin sodium* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Quinoline yellow	83.75	24.00
⋮	⋮	⋮
Mometasone furoate	>50	100.04
Atropine sulfate	>50	109.35
Escin, water-soluble	>50	123.96
Propranolol hydrochloride	>50	163.58
Magnesium hydrogen citrate	>50	204.36
Hydrocortisone	>50	224.98
Phenytoin	>50	250.77
Calcium orotate dihydrate	>50	299.96
Potassium sorbate	>50	422.23

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Saccharin sodium* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Saccharin sodium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Saccharin sodium	172110	23643	40	20170831*
Caelo	Saccharin sodium	162210	23857	39	20160811*
Caelo	Saccharin sodium	172592	24409	40	20171206*
Caelo	Saccharin sodium	19000658	25214	40	20200121*
Caelo	Saccharin sodium	21003326	26008	40	20220105*
Caelo	Saccharin sodium	23003299	27121	40	20240124*
Fagron	Saccharin sodium	13I20-B06-291654	23020	40	AR-17-FG-012457-01
Fagron	Saccharin sodium	14F30-B02-296322	23452	40	AR-17-FG-022421-01
Fagron	Saccharin sodium	14F30-B02-296322	23453	40	AR-18-FG-007117-02
Fagron	Saccharin sodium	18L06-B01-361488	25178	40	20190130
Fagron	Saccharin sodium	22K28-B09-221810	26615	40	20230112
Fagron	Saccharin sodium	22K28-B09-221810	26615SI	20	20230112

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 459 spectra of 12 reference samples from the substance/substance group *Saccharin sodium*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 503 spectra from a total of 2832 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 270 spectra of 8 reference samples from the substance/substance group *Saccharin sodium*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Saccharin sodium	15087704	22769	40
Caelo	Saccharin sodium	182104	24381	40
Caelo	Saccharin sodium	190964	24499	40
Caelo	Saccharin sodium	22003584	26489	40
Caelo	Saccharin sodium	23000898	26701	40
Caelo	Saccharin sodium	24001228	27251	40
Caelo	Saccharin sodium	21003326	26008SI†	10
Caelo	Saccharin sodium	22003584	26489SI	20

- 201 814 spectra from a total of 4038 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 435 spectra from 323 *Apo-Ident* customers from 79 batches from the substance/substance group *Saccharin sodium*.
- Among them are spectra of independent samples from 76 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Saccharin sodium		1
	Saccharin sodium	21003326011	1
	Saccharin sodium	21003326015	3
	Saccharin sodium	21003326024	5
	Saccharin sodium	2200354008	1
	Saccharin sodium	22003558008	1
	Saccharin sodium	22003584008	1
	Saccharin sodium	22003584014	2
	Saccharin sodium	23000898005	1
17270001	Saccharin sodium	17211002	1
Alliance Healtcare	Saccharin sodium	20004198009	1
Cael Sanacorp 05.02.2016	Saccharin sodium	15087703	1
Caeleo/ Krieger	Saccharin sodium	17329407	1
Caelo	Saccharin sodium		1
Caelo	Saccharin sodium	11025605	1
Caelo	Saccharin sodium	11025610	1
Caelo	Saccharin sodium	11172805	3
Caelo	Saccharin sodium	11172814	1
Caelo	Saccharin sodium	12139803	1
Caelo	Saccharin sodium	1236207	1
Caelo	Saccharin sodium	12362607	3
Caelo	Saccharin sodium	13205411	1
Caelo	Saccharin sodium	13205414	3
Caelo	Saccharin sodium	13205417	1
Caelo	Saccharin sodium	1402970	1
Caelo	Saccharin sodium	14029705	6
Caelo	Saccharin sodium	14029707	3
Caelo	Saccharin sodium	14029709	1
Caelo	Saccharin sodium	14029710	3
Caelo	Saccharin sodium	14213402	3
Caelo	Saccharin sodium	14213405	5
Caelo	Saccharin sodium	15084101	6
Caelo	Saccharin sodium	15087703	7
Caelo	Saccharin sodium	15087704	12
Caelo	Saccharin sodium	15087707	3
Caelo	Saccharin sodium	15087713	18
Caelo	Saccharin sodium	16221005	14
Caelo	Saccharin sodium	16221009	4
Caelo	Saccharin sodium	16221010	1
Caelo	Saccharin sodium	17211001	2
Caelo	Saccharin sodium	17211002	18
Caelo	Saccharin sodium	17211002P-190808-4	1
Caelo	Saccharin sodium	17211005	2
Caelo	Saccharin sodium	17329309	1
Caelo	Saccharin sodium	17329310	10
Caelo	Saccharin sodium	17329405	4
Caelo	Saccharin sodium	17329407	11

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Saccharin sodium	17329409	17
Caelo	Saccharin sodium	18210407	13
Caelo	Saccharin sodium	19000658002	12
Caelo	Saccharin sodium	19000658005	5
Caelo	Saccharin sodium	1906403	1
Caelo	Saccharin sodium	190964001	8
Caelo	Saccharin sodium	19096403	17
Caelo	Saccharin sodium	19096408	1
Caelo	Saccharin sodium	20000953001	13
Caelo	Saccharin sodium	20000953003	2
Caelo	Saccharin sodium	20000953006	6
Caelo	Saccharin sodium	20004198004	3
Caelo	Saccharin sodium	20004198005	8
Caelo	Saccharin sodium	20004198009	15
Caelo	Saccharin sodium	21003326006	6
Caelo	Saccharin sodium	21003326007	1
Caelo	Saccharin sodium	21003326011	5
Caelo	Saccharin sodium	21003326015	1
Caelo	Saccharin sodium	21003326019	6
Caelo	Saccharin sodium	21003326024	1
Caelo	Saccharin sodium	21092015A	1
Caelo	Saccharin sodium	220905(21003326011)	1
Caelo	Saccharin sodium	3414M-02206	1
Caelo	Saccharin sodium	3518E-02206	1
Caelo	Saccharin sodium	8121801	1
Caelo	Saccharin sodium	90542309	1
Caelo	Saccharin sodium	9381714	1
Caelo	Saccharin sodium	B190964001	1
Caesar & Loretz GmbH...	Saccharin sodium	21003326019	4
Caesar & Loretz GmbH...	Saccharin sodium	17329407	1
Caesar & Loretz GmbH...	Saccharin sodium	13205418	2
Caesar & Loretz GmbH...	Saccharin sodium	20004198005	1
Caesar & Loretz GmbH/AHD	Saccharin sodium	20004198005	1
Caesar & Loretz GmbH/AHD	Saccharin sodium	21003326019	1
Caesar & Loretz GmbH...	Saccharin sodium	20000953001	1
Caesar & Loretz GmbH/E	Saccharin sodium	21003326011	1
Caesar & Loretz GmbH/Gehe	Saccharin sodium	20000953	1
Caesar & Loretz GmbH...	Saccharin sodium	21003326006	1
Caesar & Loretz GmbH...	Saccharin sodium	21003326006	1
Caesar & Loretz GmbH...	Saccharin sodium	21003326024	1
Caesar & Loretz GmbH...	Saccharin sodium	19096403	2
Caesar & Loretz GmbH/Sa	Saccharin sodium	20004198004	1
Caesar & Loretz GmbH...	Saccharin sodium	20004198004	1
Caesar & Loretz GmbH...	Saccharin sodium	20004198006	1
Caesar & Loretz GmbH	Saccharin sodium	17211002	1
Caesar & Loretz GmbH	Saccharin sodium	17329310	2
Caesar & Loretz GmbH	Saccharin sodium	17329311	1
Caesar & Loretz GmbH	Saccharin sodium	17329409	1
Caesar & Loretz GmbH	Saccharin sodium	18210407	4
Caesar & Loretz GmbH	Saccharin sodium	19000658002	1
Caesar & Loretz GmbH	Saccharin sodium	190964001	3
Caesar & Loretz GmbH	Saccharin sodium	19096403	4
Caesar & Loretz GmbH	Saccharin sodium	20000953001	6
Caesar & Loretz GmbH	Saccharin sodium	20004198004	1
Caesar & Loretz GmbH	Saccharin sodium	20004198005	5
Caesar & Loretz GmbH	Saccharin sodium	20004198009	7
Caesar & Loretz GmbH	Saccharin sodium	21003326006	5
Caesar & Loretz GmbH	Saccharin sodium	21003326011	4
Caesar & Loretz GmbH	Saccharin sodium	21003326015	4
Caesar & Loretz GmbH	Saccharin sodium	21003326019	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz Hild…	Saccharin sodium	190964001	1
Caesar & Loretz Hilden	Saccharin sodium	17329407	1
Caesar & Loretz/Geil…	Saccharin sodium	20000953001	1
Caesar Loretz	Saccharin sodium	20000953001	1
Caesar&Lorenz	Saccharin sodium	19000658005	1
Caesar&loretz,Phoenix	Saccharin sodium	15084101	1
Cealo/ Noweda	Saccharin sodium	17329407	1
cealo	Saccharin sodium	15087703	1
Cealo	Saccharin sodium	17329405	1
Cealo	Saccharin sodium	19000658002	1
Euro OTC	Saccharin sodium	15087704	1
Euro OTC	Saccharin sodium	15087713	1
Fagron	Saccharin sodium	12A13-N03	2
Fagron	Saccharin sodium	12K26-N09	1
Fagron	Saccharin sodium	13D19-N01	1
Fagron	Saccharin sodium	SH349/12	1
Fargon	Saccharin sodium	12A13-NO3	1
Gehe	Saccharin sodium	18210407	2
Gehe	Saccharin sodium	21003326011	1
Gehe	Saccharin sodium	23003240002	1
Henry Lamotte/AHD	Saccharin sodium	17329405	1
Ichthyol-Gesellschaft	Saccharin sodium	16221009	1
Jenne	Saccharin sodium	15087707	1
Jenne	Saccharin sodium	22003584008	1
Kehr	Saccharin sodium	17329407	1
Nachprüfung von Nove…	Saccharin sodium	14029707	2
Noweda	Saccharin sodium	20000953001	1
Noweda	Saccharin sodium	20000953003	1
Noweda	Saccharin sodium	21003326024	1
Pharmachem	Saccharin sodium	17329407	1
Phoenix	Saccharin sodium	14F30-B02-296322	1
Phönix	Saccharin sodium	17329407	1
Phönix	Saccharin sodium	19000658002	1
Phönix	Saccharin sodium	22003584014	1
Sana 03.11.14 EK 3,95	Saccharin sodium	14029707	1
sanacorp	Saccharin sodium	13205418	1
Sanacorp	Saccharin sodium	17211002	2

- 235 632 spectra from 1515 *Apo-Ident* customers from a total of 49 180 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Saccharin sodium* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Saccharin sodium* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	459	0	152 503
Type B	0	270	0	201 814
Type C	0	435	0	235 632

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The substance/substance group *Saccharin sodium* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6928 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.7778 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 98.6207 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23020	23020	0.00	178.29
23452	23452	0.00	190.79
23453	23453	0.00	192.50
23643	23643	0.00	218.53
23857	23857	0.00	218.78
24409	24409	0.00	217.04
25178	23857	30.06	213.85
25214	25214	0.00	143.70
26008	26008	0.00	155.90
26615	23643	25.30	220.54
27121	27121	0.00	189.31

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Salbutamol sulfate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20476-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Salbutamol sulfate; Salbutamol sulphate; Salbutamoli sulfas

Special notes

When selecting the *Salbutamol sulfate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Salbutamol sulfate	4	1	0

Second-stage model

For differentiation of the substance/substance group *Salbutamol sulfate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Salbutamol sulfate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	80.45	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Salbutamol sulfate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Salbutamol sulfate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Salbutamol sulfate	13K12-N02	23232	40	1801521
Fagron	Salbutamol sulfate	17I21-B02	23993	40	20170311
Fagron	Salbutamol sulfate	22C07-B04-222382	26466	40	20220613
Fagron	Salbutamol sulfate	23H24-B03-231712	27038	40	20231116
Fagron	Salbutamol sulfate	23H24-B03-231712	27038SI	20	20231116

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 5 reference samples from the substance/substance group *Salbutamol sulfate*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 782 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 320 spectra of 8 reference samples from the substance/substance group *Salbutamol sulfate*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Salbutamol sulfate	18H21-B03-364945	26077	40
Fagron	Salbutamol sulfate	13K12-N02	21691	60
Fagron	Salbutamol sulfate	13K12-N02	23231	40
Fagron	Salbutamol sulfate	13K12-N02	23454	40
Fagron	Salbutamol sulfate	13K12-N02	23455	40
Fagron	Salbutamol sulfate	13K12-N02	23755	40
Fagron	Salbutamol sulfate	13K12-N02	23756	40
Fagron	Salbutamol sulfate	18H21-B03-364945	26077SI	20

- 201 764 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Salbutamol sulfate*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Noweda	Salbutamol sulfate	13K12-N02	1

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Salbutamol sulfate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Salbutamol sulfate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	180	0	152 782
Type B	0	320	0	201 764
Type C	0	1	0	236 066

The substance/substance group *Salbutamol sulfate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.1250 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
23232	23232	0.00	260.02
23993	23232	42.86	257.56
26466	23232	38.67	265.54
27038	23232	37.12	267.38

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Salicylic acid**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20015-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Salicylic acid; Acidum salicylicum

Special notes

When selecting the *Salicylic acid* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Salicylic acid	9	23	577

Second-stage model

For differentiation of the substance/substance group *Salicylic acid* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Salicylic acid* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Dithranol	136.91	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Salicylic acid* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Salicylic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Salicylic acid	13344002	21436	60	20131029
Caelo	Salicylic acid	13344018	21760	60	20131020
Caelo	Salicylic acid	160109	22443	60	20160229*
Caelo	Salicylic acid	22001526	26113	40	20220516*
Caelo	Salicylic acid	22001526	26113SI	20	20220516*
Euro OTC	Salicylic acid	1110020-01	20696	40	20120125
Euro OTC	Salicylic acid	1509007	21906	60	20150929*
Euro OTC	Salicylic acid	2101028	25543	40	20210304*
Fagron	Salicylic acid	16I15-B08-333932	23592	40	20170210
Fagron	Salicylic acid	190263	24591	40	20190121

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 460 spectra of 10 reference samples from the substance/substance group *Salicylic acid*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 502 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1120 spectra of 31 reference samples from the substance/substance group *Salicylic acid*.

- Among them are spectra of independent samples from 23 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Salicylic acid	160500	22448	60
Caelo	Salicylic acid	171333	23277	40
Caelo	Salicylic acid	173015	23827	40
Caelo	Salicylic acid	182300	24236	40
Caelo	Salicylic acid	192209	24883	40
Caelo	Salicylic acid	21003008	25857	50
Caelo	Salicylic acid	22001524	26103	40
Caelo	Salicylic acid	22001528	26104	40
Caelo	Salicylic acid	22001529	26105	40
Caelo	Salicylic acid	22001534	26106	40
Caelo	Salicylic acid	24000004	27235	40
Euro OTC	Salicylic acid	1605023	22685	40
Euro OTC	Salicylic acid	1707009	23556	40
Euro OTC	Salicylic acid	1801042	23968	40
Euro OTC	Salicylic acid	1901015	24471	40
Euro OTC	Salicylic acid	1910018	24925	40
Euro OTC	Salicylic acid	2108024	25821	50
Euro OTC	Salicylic acid	2201044	25950	40
Euro OTC	Salicylic acid	2208003	26280	40
Euro OTC	Salicylic acid	2308012	26872	40
Euro OTC	Salicylic acid	2311012	27154	40
Euro OTC	Salicylic acid	2407001	27290	40
Fagron	Salicylic acid	22E12-B05-227887	26609	40
Caelo	Salicylic acid	21003008	25857SI	10
Caelo	Salicylic acid	22001524	26103SI	20
Caelo	Salicylic acid	22001528	26104SI	20
Caelo	Salicylic acid	22001529	26105SI	20
Caelo	Salicylic acid	22001534	26106SI	20
Euro OTC	Salicylic acid	2108024	25821SI	10

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Salicylic acid	2201044	25950SI	40
Euro OTC	Salicylic acid	2208003	26280SI	20

- 200 964 spectra from a total of 4022 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4307 spectra from 1237 *Apo-Ident* customers from 598 batches from the substance/substance group *Salicylic acid*.
- Among them are spectra of independent samples from 572 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Salicylic acid	20003823016	3
	Salicylic acid	20004424015	2
	Salicylic acid	21003008003	1
	Salicylic acid	21003008015	1
	Salicylic acid	21003008016	10
	Salicylic acid	21003008017	1
	Salicylic acid	2100300816	1
	Salicylic acid	2101028-01	1
	Salicylic acid	22001528001	1
	Salicylic acid	22001528002	4
	Salicylic acid	22001528003	2
	Salicylic acid	2200152802	1
	Salicylic acid	22001529002	18
	Salicylic acid	22001529003	2
	Salicylic acid	220015298002	1
	Salicylic acid	22001534003	12
	Salicylic acid	22001534004	3
	Salicylic acid	22001534007	1
	Salicylic acid	2200159002	1
	Salicylic acid	2201044-2	1
	Salicylic acid	2208003-01	4
	Salicylic acid	2208003-02	9
	Salicylic acid	22D07-B03-221811	1
	Salicylic acid	22DS07-B03-221811	1
	Salicylic acid	22j26-b06-227888	1
	Salicylic acid	22J26-B06-227888	1
	Salicylic acid	22J26-B06-2278888	1
	Salicylic acid	23002014002	1
	Salicylic acid	23002014003	12
	Salicylic acid	2308012-01	4
	Salicylic acid	2311012-01	1
	Salicylic acid	2388012-01	1
	Salicylic acid	23B01-B01-232363	1
	Salicylic acid	24000043001	6
	Salicylic acid	B03-2218101	1
14076202	Salicylic acid		1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
ACM	Salicylic acid	KNC0461J15	1
AHC	Salicylic acid	20004424011	1
AHC	Salicylic acid	22001529002	1
AHD 22.07.14	Salicylic acid	134002	1
AHD	Salicylic acid	13344002	1
AHD	Salicylic acid	1509007-01	1
AHD	Salicylic acid	192209003	1
AHD	Salicylic acid	22001524003	1
AHD	Salicylic acid	22001528002	2
AHD	Salicylic acid	22001529003	1
AHD	Salicylic acid	22001534007	1
Alliance 19.12.12	Salicylic acid	11311906	1
Alliance Healthcare	Salicylic acid	12036215	2
Alliance Healthcare	Salicylic acid	12036216	1
Alliance Healthcare	Salicylic acid	15211808	1
Alliance	Salicylic acid	21003008016	1
Anzag/Anzag 11.09.18	Salicylic acid	18F05-B02-350586	1
Anzag/Henry Lamotte	Salicylic acid	1334018	1
Anzag	Salicylic acid	1303020-01	2
Anzag	Salicylic acid	16050014	1
apo ident	Salicylic acid	1605023-01	1
apomix	Salicylic acid	2108024-01	1
Bombastus	Salicylic acid	12036223	1
Bombastus	Salicylic acid	12323403	1
Bombastus	Salicylic acid	14L02-B02-303557	1
Bombastus	Salicylic acid	16050017	1
Bombastus	Salicylic acid	1605023-01	1
Bombastus	Salicylic acid	17301505	1
Caaelo	Salicylic acid	14336911	1
Caela	Salicylic acid	16312001	1
Caelo	Salicylic acid		8
Caelo	Salicylic acid	10001612	1
Caelo	Salicylic acid	10112014B	1
Caelo	Salicylic acid	102455-0001	1
Caelo	Salicylic acid	10291803	1
Caelo	Salicylic acid	10291817	1
Caelo	Salicylic acid	10355907	1
Caelo	Salicylic acid	10355911	2
Caelo	Salicylic acid	10355912	1
Caelo	Salicylic acid	10355916	1
Caelo	Salicylic acid	1045	1
Caelo	Salicylic acid	11197103	1
Caelo	Salicylic acid	11197106	1
Caelo	Salicylic acid	11197117	1
Caelo	Salicylic acid	11197118	1
Caelo	Salicylic acid	11197123	4
Caelo	Salicylic acid	11311902	2
Caelo	Salicylic acid	11311903	1
Caelo	Salicylic acid	11311905	1
Caelo	Salicylic acid	11311906	2
Caelo	Salicylic acid	11311910	2
Caelo	Salicylic acid	11311917	4
Caelo	Salicylic acid	11311922	11
Caelo	Salicylic acid	11311923	2
Caelo	Salicylic acid	117027-2	1
Caelo	Salicylic acid	12036202	3
Caelo	Salicylic acid	12036208	1
Caelo	Salicylic acid	12036209	4
Caelo	Salicylic acid	12036210	3
Caelo	Salicylic acid	12036211	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Salicylic acid	12036215	2
Caelo	Salicylic acid	12036216	5
Caelo	Salicylic acid	12036217	2
Caelo	Salicylic acid	12036223	8
Caelo	Salicylic acid	12036225	4
Caelo	Salicylic acid	12036226	7
Caelo	Salicylic acid	12036315	1
Caelo	Salicylic acid	12134702	12
Caelo	Salicylic acid	12134707	6
Caelo	Salicylic acid	12134709	23
Caelo	Salicylic acid	12134710	1
Caelo	Salicylic acid	12134711	10
Caelo	Salicylic acid	12134712	4
Caelo	Salicylic acid	12134713	1
Caelo	Salicylic acid	12134714	16
Caelo	Salicylic acid	12134715	7
Caelo	Salicylic acid	12134717	9
Caelo	Salicylic acid	12134719	4
Caelo	Salicylic acid	12134720	8
Caelo	Salicylic acid	12134721	2
Caelo	Salicylic acid	12134722	4
Caelo	Salicylic acid	123134712	1
Caelo	Salicylic acid	12323401	1
Caelo	Salicylic acid	12323402	2
Caelo	Salicylic acid	12323403	3
Caelo	Salicylic acid	1234	1
Caelo	Salicylic acid	1234709	1
Caelo	Salicylic acid	12374204	1
Caelo	Salicylic acid	12374205	8
Caelo	Salicylic acid	12374207	6
Caelo	Salicylic acid	12374207-3454311172	1
Caelo	Salicylic acid	12374208	2
Caelo	Salicylic acid	12374210	3
Caelo	Salicylic acid	12374211	18
Caelo	Salicylic acid	12374212	2
Caelo	Salicylic acid	12374213	11
Caelo	Salicylic acid	1274210	1
Caelo	Salicylic acid	12H10-N08	5
Caelo	Salicylic acid	1303020-01	2
Caelo	Salicylic acid	13032014A	1
Caelo	Salicylic acid	13101707	1
Caelo	Salicylic acid	1310516	1
Caelo	Salicylic acid	13344002	20
Caelo	Salicylic acid	13344003	10
Caelo	Salicylic acid	13344013	11
Caelo	Salicylic acid	13344014	6
Caelo	Salicylic acid	13344018	19
Caelo	Salicylic acid	13344020	17
Caelo	Salicylic acid	1334403	1
Caelo	Salicylic acid	133454002	1
Caelo	Salicylic acid	13B14-No1	1
Caelo	Salicylic acid	13H01-N01	1
Caelo	Salicylic acid	13H01-N04	2
Caelo	Salicylic acid	1406027	1
Caelo	Salicylic acid	140602701	1
Caelo	Salicylic acid	1406027-02	3
Caelo	Salicylic acid	14076201	1
Caelo	Salicylic acid	14076202	6
Caelo	Salicylic acid	14076203	7
Caelo	Salicylic acid	14076204	11

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Salicylic acid	14076206	7
Caelo	Salicylic acid	14076207	10
Caelo	Salicylic acid	14076211	1
Caelo	Salicylic acid	14076212	1
Caelo	Salicylic acid	14300801	8
Caelo	Salicylic acid	14300802	6
Caelo	Salicylic acid	14300804	7
Caelo	Salicylic acid	14300805	11
Caelo	Salicylic acid	14300806	1
Caelo	Salicylic acid	14300808	1
Caelo	Salicylic acid	14300809	12
Caelo	Salicylic acid	1430802	1
Caelo	Salicylic acid	1433620	1
Caelo	Salicylic acid	14336904	2
Caelo	Salicylic acid	14336905	15
Caelo	Salicylic acid	14336906	4
Caelo	Salicylic acid	14336907	26
Caelo	Salicylic acid	14336908	3
Caelo	Salicylic acid	14336911	24
Caelo	Salicylic acid	14336912	9
Caelo	Salicylic acid	14336919	24
Caelo	Salicylic acid	14336920	24
Caelo	Salicylic acid	14336921	1
Caelo	Salicylic acid	14E26-B04-294622	1
Caelo	Salicylic acid	14L02-B02-303558	1
Caelo	Salicylic acid	15081601	1
Caelo	Salicylic acid	15084401	4
Caelo	Salicylic acid	15084403	7
Caelo	Salicylic acid	15084404	3
Caelo	Salicylic acid	1509007-01	1
Caelo	Salicylic acid	1509007-02	2
Caelo	Salicylic acid	151224/1	1
Caelo	Salicylic acid	152117304	1
Caelo	Salicylic acid	15211803	1
Caelo	Salicylic acid	15211806	2
Caelo	Salicylic acid	15211807	2
Caelo	Salicylic acid	15211808	10
Caelo	Salicylic acid	15211809	14
Caelo	Salicylic acid	15211810	10
Caelo	Salicylic acid	15217301	6
Caelo	Salicylic acid	15217302	19
Caelo	Salicylic acid	15217303	9
Caelo	Salicylic acid	15217304	7
Caelo	Salicylic acid	15217305	6
Caelo	Salicylic acid	15217308	8
Caelo	Salicylic acid	15217309	1
Caelo	Salicylic acid	16/15-B08-332098	1
Caelo	Salicylic acid	1600917	1
Caelo	Salicylic acid	16010901	5
Caelo	Salicylic acid	16010901s	1
Caelo	Salicylic acid	16010903	17
Caelo	Salicylic acid	16010904	12
Caelo	Salicylic acid	16010905	11
Caelo	Salicylic acid	16010906	17
Caelo	Salicylic acid	16010907	6
Caelo	Salicylic acid	16010908	3
Caelo	Salicylic acid	16010910	17
Caelo	Salicylic acid	16010911	4
Caelo	Salicylic acid	16010912	4
Caelo	Salicylic acid	160109123	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Salicylic acid	16010913	18
Caelo	Salicylic acid	16010916	5
Caelo	Salicylic acid	16010917	16
Caelo	Salicylic acid	16010918	11
Caelo	Salicylic acid	16010921	3
Caelo	Salicylic acid	16010922	16
Caelo	Salicylic acid	16010923	7
Caelo	Salicylic acid	16010972	1
Caelo	Salicylic acid	1601916	1
Caelo	Salicylic acid	160405AS	1
Caelo	Salicylic acid	160500004	3
Caelo	Salicylic acid	16050003	2
Caelo	Salicylic acid	16050004	18
Caelo	Salicylic acid	16050005	11
Caelo	Salicylic acid	16050006	3
Caelo	Salicylic acid	16050011	15
Caelo	Salicylic acid	16050012	16
Caelo	Salicylic acid	16050013	26
Caelo	Salicylic acid	16050014	30
Caelo	Salicylic acid	16050016	1
Caelo	Salicylic acid	16050017	18
Caelo	Salicylic acid	1605023-01	1
Caelo	Salicylic acid	1605023-02	2
Caelo	Salicylic acid	16072014A	1
Caelo	Salicylic acid	163120	1
Caelo	Salicylic acid	16312001	24
Caelo	Salicylic acid	16312003	12
Caelo	Salicylic acid	16312004	2
Caelo	Salicylic acid	16312005	30
Caelo	Salicylic acid	16312008	1
Caelo	Salicylic acid	16312009	13
Caelo	Salicylic acid	16312010	25
Caelo	Salicylic acid	16312012	4
Caelo	Salicylic acid	16E02-B09-325355	1
Caelo	Salicylic acid	16I15-B08	1
Caelo	Salicylic acid	16i15-B08-0001	1
Caelo	Salicylic acid	170301506	1
Caelo	Salicylic acid	170509AS/16050012	1
Caelo	Salicylic acid	17051803	1
Caelo	Salicylic acid	1707009-01	4
Caelo	Salicylic acid	170700902	1
Caelo	Salicylic acid	17123301	1
Caelo	Salicylic acid	1713301	1
Caelo	Salicylic acid	1713307	1
Caelo	Salicylic acid	17133301	26
Caelo	Salicylic acid	17133303	23
Caelo	Salicylic acid	17133304	4
Caelo	Salicylic acid	17133307	59
Caelo	Salicylic acid	171333207	1
Caelo	Salicylic acid	1714Q1045	1
Caelo	Salicylic acid	17301502	25
Caelo	Salicylic acid	17301503	28
Caelo	Salicylic acid	17301504	5
Caelo	Salicylic acid	17301505	27
Caelo	Salicylic acid	17301506	57
Caelo	Salicylic acid	17301507	21
Caelo	Salicylic acid	17301509	36
Caelo	Salicylic acid	17301511	11
Caelo	Salicylic acid	17301512	31
Caelo	Salicylic acid	17301512/P-04041921	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Salicylic acid	17301612	1
Caelo	Salicylic acid	1738980	1
Caelo	Salicylic acid	17901506	1
Caelo	Salicylic acid	17C21-B09-337172	2
Caelo	Salicylic acid	17C21-B09-337173	1
Caelo	Salicylic acid	180050009	1
Caelo	Salicylic acid	180104201	1
Caelo	Salicylic acid	1801042-01	5
Caelo	Salicylic acid	18050002	12
Caelo	Salicylic acid	18050005	1
Caelo	Salicylic acid	18050006	38
Caelo	Salicylic acid	18050007	19
Caelo	Salicylic acid	18050009	27
Caelo	Salicylic acid	1805009	1
Caelo	Salicylic acid	18121412	1
Caelo	Salicylic acid	181473001	9
Caelo	Salicylic acid	18147302	31
Caelo	Salicylic acid	18147303	13
Caelo	Salicylic acid	18147305	1
Caelo	Salicylic acid	18147307	1
Caelo	Salicylic acid	18147308	19
Caelo	Salicylic acid	18147310	26
Caelo	Salicylic acid	18147314	40
Caelo	Salicylic acid	18147315	5
Caelo	Salicylic acid	18147317	17
Caelo	Salicylic acid	18147321	43
Caelo	Salicylic acid	182300002P-200609-3	1
Caelo	Salicylic acid	18230002	3
Caelo	Salicylic acid	18230002P-200806-1	1
Caelo	Salicylic acid	18230004	18
Caelo	Salicylic acid	18230004/P-26041921	1
Caelo	Salicylic acid	18230007	46
Caelo	Salicylic acid	18230009	15
Caelo	Salicylic acid	18230010	1
Caelo	Salicylic acid	18230013	4
Caelo	Salicylic acid	18306909	1
Caelo	Salicylic acid	18E24-B03-354310	1
Caelo	Salicylic acid	18E24-B03-354311	3
Caelo	Salicylic acid	18F05-B02-352210	2
Caelo	Salicylic acid	1901015-01	2
Caelo	Salicylic acid	190263	2
Caelo	Salicylic acid	190264	2
Caelo	Salicylic acid	190312004	1
Caelo	Salicylic acid	1906105	1
Caelo	Salicylic acid	190612001	26
Caelo	Salicylic acid	190612003	1
Caelo	Salicylic acid	190612004	37
Caelo	Salicylic acid	19061201	3
Caelo	Salicylic acid	19061202	13
Caelo	Salicylic acid	19061205	38
Caelo	Salicylic acid	19061206	33
Caelo	Salicylic acid	19062001	1
Caelo	Salicylic acid	1906612001	1
Caelo	Salicylic acid	1910018-01	1
Caelo	Salicylic acid	1910018-03	1
Caelo	Salicylic acid	1913Q-01045	1
Caelo	Salicylic acid	1922090003	1
Caelo	Salicylic acid	192209001	29
Caelo	Salicylic acid	192209003	29
Caelo	Salicylic acid	192209006	9

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Salicylic acid	1961206	1
Caelo	Salicylic acid	200000147004	1
Caelo	Salicylic acid	20000146005	13
Caelo	Salicylic acid	20000147002	25
Caelo	Salicylic acid	20000147002/4720	1
Caelo	Salicylic acid	20000147004	27
Caelo	Salicylic acid	20000147006	20
Caelo	Salicylic acid	200004424004	1
Caelo	Salicylic acid	200004424012	1
Caelo	Salicylic acid	20003823008	31
Caelo	Salicylic acid	20003823010	7
Caelo	Salicylic acid	20003823011	2
Caelo	Salicylic acid	20003823014	5
Caelo	Salicylic acid	20003823015	1
Caelo	Salicylic acid	20003823016	10
Caelo	Salicylic acid	2000442004	1
Caelo	Salicylic acid	20004421006	1
Caelo	Salicylic acid	20004424001	15
Caelo	Salicylic acid	20004424004	28
Caelo	Salicylic acid	20004424006	27
Caelo	Salicylic acid	20004424007	3
Caelo	Salicylic acid	20004424009	1
Caelo	Salicylic acid	20004424010	26
Caelo	Salicylic acid	20004424011	8
Caelo	Salicylic acid	20004424012	20
Caelo	Salicylic acid	20004424015	8
Caelo	Salicylic acid	2004424001	1
Caelo	Salicylic acid	20111306	1
Caelo	Salicylic acid	20151112-4	1
Caelo	Salicylic acid	2017-11-23-AXILU	1
Caelo	Salicylic acid	20270312-2	1
Caelo	Salicylic acid	207102017/16050017	1
Caelo	Salicylic acid	21000488001	14
Caelo	Salicylic acid	21003008001	5
Caelo	Salicylic acid	21003008003	5
Caelo	Salicylic acid	21003008004	17
Caelo	Salicylic acid	21003008009	8
Caelo	Salicylic acid	21003008010	8
Caelo	Salicylic acid	21003008015	1
Caelo	Salicylic acid	21003008016	2
Caelo	Salicylic acid	21003008017	1
Caelo	Salicylic acid	2100488001	1
Caelo	Salicylic acid	2101028-01	1
Caelo	Salicylic acid	2103008004	1
Caelo	Salicylic acid	216E-03750	1
Caelo	Salicylic acid	220001524003	1
Caelo	Salicylic acid	22001158002	1
Caelo	Salicylic acid	22001524003	23
Caelo	Salicylic acid	22001528001	6
Caelo	Salicylic acid	22001528002	8
Caelo	Salicylic acid	22001534003	2
Caelo	Salicylic acid	23002014002	1
Caelo	Salicylic acid	23002014003	1
Caelo	Salicylic acid	23071510	1
Caelo	Salicylic acid	25041304	1
Caelo	Salicylic acid	2882	1
Caelo	Salicylic acid	31012023-01	1
Caelo	Salicylic acid	3111J01045	1
Caelo	Salicylic acid	3344003	1
Caelo	Salicylic acid	3601413011-12374211	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Salicylic acid	3816Q-01045	1
Caelo	Salicylic acid	3944581	1
Caelo	Salicylic acid	3948107	1
Caelo	Salicylic acid	4010Q-01045	1
Caelo	Salicylic acid	415593	1
Caelo	Salicylic acid	4515E-01045	1
Caelo	Salicylic acid	501171101	1
Caelo	Salicylic acid	5112V01405	1
Caelo	Salicylic acid	54168742	1
Caelo	Salicylic acid	6/20151706	1
Caelo	Salicylic acid	7071403	1
Caelo	Salicylic acid	72(18230009)	1
Caelo	Salicylic acid	73(20004424001)	1
Caelo	Salicylic acid	7466	1
Caelo	Salicylic acid	8170717	1
Caelo	Salicylic acid	8715	1
Caelo	Salicylic acid	9091301	1
Caelo	Salicylic acid	9112013A	1
Caelo	Salicylic acid	9220715	1
Caelo	Salicylic acid	922090031	1
Caelo	Salicylic acid	922090061	1
Caelo	Salicylic acid	A-100513-1	1
Caelo	Salicylic acid	A320004424007	1
Caelo	Salicylic acid	RAS1135100	1
Caelo	Salicylic acid	RAS1703500	1
Caelo	Salicylic acid	test	1
Caelo	Salicylic acid	Validierungsmessung	1
Caeo	Salicylic acid	1010905	1
Caeolo/Alliance	Salicylic acid	21003008010	1
Caesaer/Jenne	Salicylic acid	18050006	1
Caesar & Loretz GmbH...	Salicylic acid	22001524003	1
Caesar & Loretz GmbH...	Salicylic acid	18147308	1
Caesar & Loretz GmbH...	Salicylic acid	18147310	1
Caesar & Loretz GmbH...	Salicylic acid	22001524003	2
Caesar & Loretz GmbH...	Salicylic acid	17301512	1
Caesar & Loretz GmbH...	Salicylic acid	18050006	2
Caesar & Loretz GmbH...	Salicylic acid	20000147004	1
Caesar & Loretz GmbH...	Salicylic acid	20003823016	1
Caesar & Loretz GmbH...	Salicylic acid	18147321	1
Caesar & Loretz GmbH...	Salicylic acid	18147314	3
Caesar & Loretz GmbH...	Salicylic acid	190612004	1
Caesar & Loretz GmbH...	Salicylic acid	19061206	1
Caesar & Loretz GmbH...	Salicylic acid	11311904	1
Caesar & Loretz GmbH...	Salicylic acid	12134714	1
Caesar & Loretz GmbH...	Salicylic acid	20004424001	1
Caesar & Loretz GmbH...	Salicylic acid	11311917	1
Caesar & Loretz GmbH/ AHD	Salicylic acid	18230004	1
Caesar & Loretz GmbH...	Salicylic acid	192209001	1
Caesar & Loretz GmbH...	Salicylic acid	190612004	1
Caesar & Loretz GmbH...	Salicylic acid	18147314	1
Caesar & Loretz GmbH...	Salicylic acid	20004424011	1
Caesar & Loretz GmbH...	Salicylic acid	18147314	1
Caesar & Loretz GmbH/AEP	Salicylic acid	18230009	1
Caesar & Loretz GmbH/AHD	Salicylic acid	18147321	1
Caesar & Loretz GmbH/AHD	Salicylic acid	20004424004	1
Caesar & Loretz GmbH/AHD	Salicylic acid	21003008004	1
Caesar & Loretz GmbH...	Salicylic acid	20004424004	3
Caesar & Loretz GmbH...	Salicylic acid	18050006	1
Caesar & Loretz GmbH/G	Salicylic acid	20004424004	1
Caesar & Loretz GmbH/Gehe	Salicylic acid	18147308	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Gehe	Salicylic acid	192209001	1
Caesar & Loretz GmbH/GEHE	Salicylic acid	192209006	1
Caesar & Loretz GmbH/Gehe	Salicylic acid	20000146	1
Caesar & Loretz GmbH/Gehe	Salicylic acid	20003823008	1
Caesar & Loretz GmbH/Gehe	Salicylic acid	20003823014	1
Caesar & Loretz GmbH/Gehe	Salicylic acid	20004424006	1
Caesar & Loretz GmbH/Gehe	Salicylic acid	20004424011	1
Caesar & Loretz GmbH/Gehe	Salicylic acid	21000488001	2
Caesar & Loretz GmbH/Gehe	Salicylic acid	21003008001	1
Caesar & Loretz GmbH/Gehe	Salicylic acid	22001528001	1
Caesar & Loretz GmbH...	Salicylic acid	192209001	2
Caesar & Loretz GmbH...	Salicylic acid	20004424010	2
Caesar & Loretz GmbH...	Salicylic acid	22001528002	2
Caesar & Loretz GmbH/Gö	Salicylic acid	18147321	1
Caesar & Loretz GmbH...	Salicylic acid	18147314	1
Caesar & Loretz GmbH...	Salicylic acid	20003823008	1
Caesar & Loretz GmbH...	Salicylic acid	18147308	1
Caesar & Loretz GmbH...	Salicylic acid	20004424011	1
Caesar & Loretz GmbH/Kehr	Salicylic acid	19061205	1
Caesar & Loretz GmbH/Kehr	Salicylic acid	192209006	1
Caesar & Loretz GmbH/Kehr	Salicylic acid	2100308015	1
Caesar & Loretz GmbH/Now.	Salicylic acid	18147321	1
Caesar & Loretz GmbH...	Salicylic acid	190612004	1
Caesar & Loretz GmbH...	Salicylic acid	19061206	1
Caesar & Loretz GmbH...	Salicylic acid	192209003	1
Caesar & Loretz GmbH...	Salicylic acid	20004424004	1
Caesar & Loretz GmbH...	Salicylic acid	20004424015	1
Caesar & Loretz GmbH/Otto	Salicylic acid	19061202	1
Caesar & Loretz GmbH...	Salicylic acid	22001524003	1
Caesar & Loretz GmbH...	Salicylic acid	22001528002	2
Caesar & Loretz GmbH...	Salicylic acid	18147321	2
Caesar & Loretz GmbH...	Salicylic acid	18230007	1
Caesar & Loretz GmbH...	Salicylic acid	19061206	1
Caesar & Loretz GmbH...	Salicylic acid	20004424001	1
Caesar & Loretz GmbH...	Salicylic acid	20004424006	2
Caesar & Loretz GmbH...	Salicylic acid	22001528001	2
Caesar & Loretz GmbH...	Salicylic acid	20000146005	1
Caesar & Loretz GmbH...	Salicylic acid	20000147002	1
Caesar & Loretz GmbH...	Salicylic acid	20000147004	1
Caesar & Loretz GmbH...	Salicylic acid	20000147006	1
Caesar & Loretz GmbH...	Salicylic acid	18230009	1
Caesar & Loretz GmbH	Salicylic acid	11311922	1
Caesar & Loretz GmbH	Salicylic acid	13344003	1
Caesar & Loretz GmbH	Salicylic acid	14300809	1
Caesar & Loretz GmbH	Salicylic acid	16312001	1
Caesar & Loretz GmbH	Salicylic acid	16312005	1
Caesar & Loretz GmbH	Salicylic acid	16312012	1
Caesar & Loretz GmbH	Salicylic acid	17133301	1
Caesar & Loretz GmbH	Salicylic acid	17301509	1
Caesar & Loretz GmbH	Salicylic acid	17301512	9
Caesar & Loretz GmbH	Salicylic acid	18050002	1
Caesar & Loretz GmbH	Salicylic acid	18050006	3
Caesar & Loretz GmbH	Salicylic acid	18050007	2
Caesar & Loretz GmbH	Salicylic acid	18050009	4
Caesar & Loretz GmbH	Salicylic acid	18147302	9
Caesar & Loretz GmbH	Salicylic acid	18147303	6
Caesar & Loretz GmbH	Salicylic acid	18147308	5
Caesar & Loretz GmbH	Salicylic acid	18147310	3
Caesar & Loretz GmbH	Salicylic acid	18147313	1
Caesar & Loretz GmbH	Salicylic acid	18147314	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Salicylic acid	18147315	2
Caesar & Loretz GmbH	Salicylic acid	18147317	3
Caesar & Loretz GmbH	Salicylic acid	18147321	17
Caesar & Loretz GmbH	Salicylic acid	18147322	1
Caesar & Loretz GmbH	Salicylic acid	18230004	3
Caesar & Loretz GmbH	Salicylic acid	18230007	7
Caesar & Loretz GmbH	Salicylic acid	18230009	3
Caesar & Loretz GmbH	Salicylic acid	18230013	2
Caesar & Loretz GmbH	Salicylic acid	1847302	1
Caesar & Loretz GmbH	Salicylic acid	190612001	9
Caesar & Loretz GmbH	Salicylic acid	190612003	1
Caesar & Loretz GmbH	Salicylic acid	190612004	6
Caesar & Loretz GmbH	Salicylic acid	19061201	1
Caesar & Loretz GmbH	Salicylic acid	19061202	1
Caesar & Loretz GmbH	Salicylic acid	19061205	12
Caesar & Loretz GmbH	Salicylic acid	19061206	9
Caesar & Loretz GmbH	Salicylic acid	192209001	8
Caesar & Loretz GmbH	Salicylic acid	192209003	9
Caesar & Loretz GmbH	Salicylic acid	192209004	2
Caesar & Loretz GmbH	Salicylic acid	192209006	5
Caesar & Loretz GmbH	Salicylic acid	20000146004	4
Caesar & Loretz GmbH	Salicylic acid	20000146005	5
Caesar & Loretz GmbH	Salicylic acid	20000147002	15
Caesar & Loretz GmbH	Salicylic acid	20000147004	14
Caesar & Loretz GmbH	Salicylic acid	20000147006	11
Caesar & Loretz GmbH	Salicylic acid	2000147002	1
Caesar & Loretz GmbH	Salicylic acid	20003823008	11
Caesar & Loretz GmbH	Salicylic acid	20003823010	5
Caesar & Loretz GmbH	Salicylic acid	20003823011	1
Caesar & Loretz GmbH	Salicylic acid	20003823014	4
Caesar & Loretz GmbH	Salicylic acid	20003823015	1
Caesar & Loretz GmbH	Salicylic acid	20003823016	3
Caesar & Loretz GmbH	Salicylic acid	20004424001	7
Caesar & Loretz GmbH	Salicylic acid	20004424002	2
Caesar & Loretz GmbH	Salicylic acid	20004424004	5
Caesar & Loretz GmbH	Salicylic acid	20004424006	4
Caesar & Loretz GmbH	Salicylic acid	20004424007	4
Caesar & Loretz GmbH	Salicylic acid	20004424009	1
Caesar & Loretz GmbH	Salicylic acid	20004424010	5
Caesar & Loretz GmbH	Salicylic acid	20004424011	2
Caesar & Loretz GmbH	Salicylic acid	20004424012	3
Caesar & Loretz GmbH	Salicylic acid	20004424013	4
Caesar & Loretz GmbH	Salicylic acid	20004424015	2
Caesar & Loretz GmbH	Salicylic acid	21003008001	4
Caesar & Loretz GmbH	Salicylic acid	21003008003	5
Caesar & Loretz GmbH	Salicylic acid	21003008004	15
Caesar & Loretz GmbH	Salicylic acid	21003008009	3
Caesar & Loretz GmbH	Salicylic acid	21003008010	7
Caesar & Loretz GmbH	Salicylic acid	21003008015	1
Caesar & Loretz GmbH	Salicylic acid	21003008016	2
Caesar & Loretz GmbH	Salicylic acid	22001088004	1
Caesar & Loretz GmbH	Salicylic acid	22001524003	1
Caesar & Loretz GmbH	Salicylic acid	22001528001	4
Caesar & Loretz GmbH	Salicylic acid	22001528002	5
Caesar & Loretz Hild…	Salicylic acid	192209001	1
Caesar & Loretz Hilden	Salicylic acid	17301512	1
Caesar & Loretz Hilden	Salicylic acid	18230007	1
Caesar & Loretz Hilden	Salicylic acid	19061205	1
Caesar & Loretz Hilden	Salicylic acid	192209003	1
Caesar & Loretz/Gehe	Salicylic acid	20000147004	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz/Geil…	Salicylic acid	17301509	1
Caesar & Loretz/Sanacorp	Salicylic acid	17301503	1
Caesar & Loretz	Salicylic acid	17301502	1
Caesar & Loretz	Salicylic acid	21003008001	1
Caesar & Loretz	Salicylic acid	21003008009	1
Caesar / Ebert & Jacobi	Salicylic acid	16312010	2
Caesar Loretz	Salicylic acid	192209001	1
Caesar u. Loretz GmbH	Salicylic acid	190612004	1
Caesar u. Loretz GmbH	Salicylic acid	192209006	1
Caesar und Loretz GmbH	Salicylic acid	16312003	1
Caesar&Lorenz / Gehe	Salicylic acid	18230004	1
Caesar&Lorenz	Salicylic acid	20004424006	1
Caesar&Loretz Anzag	Salicylic acid	14300804	2
Caesar&Loretz GmbH,1…	Salicylic acid	16312001	1
Caesar&Loretz GmbH/Anzag	Salicylic acid	12374204	1
Caesar&Loretz GmbH/Anzag	Salicylic acid	14076203	2
Caesar&Loretz GmbH/S…	Salicylic acid	15217301	1
Caesar&Loretz GmbH/S…	Salicylic acid	18230009	1
Caesar&loretz,Anzag	Salicylic acid	12036211	1
Caesar&loretz,Phoenix	Salicylic acid	11197104	1
Caesar&loretz,Phoenix	Salicylic acid	14076212	1
Caesar&loretz,Phoenix	Salicylic acid	9220710	1
Caesar&Loretz/AHD	Salicylic acid	15211808	1
Caesar&Loretz	Salicylic acid	18230007	1
caesar	Salicylic acid	15217301	1
Caleo/n	Salicylic acid	17301502	1
Caleo/Phoenix	Salicylic acid	21003008003	1
Caolo- Noweda	Salicylic acid	14300809	2
carlo	Salicylic acid	12134714	2
Cealo/Gehe	Salicylic acid	20000147004	1
Cealo/Noweda	Salicylic acid	17301509	1
Cealo/Sanacorp	Salicylic acid	17133307	1
Cealo/Sanacorp	Salicylic acid	20000147006	1
Cealo	Salicylic acid	15211806	1
cealo	Salicylic acid	18050007	1
Celo/ Sanacorp	Salicylic acid	16010908	1
Delta	Salicylic acid	17133303	1
E Plus	Salicylic acid	16I15-B08-333932	1
Ebert 24.08.16	Salicylic acid	16010903	1
Ebert & Jacobi	Salicylic acid	16010923	1
EuRho 001	Salicylic acid	1509007-02	1
Eurho/ Noweda	Salicylic acid	1901015-01	1
Eurho/ Noweda	Salicylic acid	1901015-03	1
EuRho/ Phönix	Salicylic acid	RAS1730100	1
EuRho/Gehe	Salicylic acid	1910018-01	1
EuRho/Noweda	Salicylic acid	1910018-02	1
Eurho/Phoenix	Salicylic acid	13B14-N01	2
EuRho/VDL	Salicylic acid	1801042-01	1
EuRho	Salicylic acid		1
EuRho	Salicylic acid	1206007-01	2
EuRho	Salicylic acid	1303020-01	1
EuRho	Salicylic acid	1406027-01	2
EuRho	Salicylic acid	1406027-02	1
EuRho	Salicylic acid	1707009-01	2
EuRho	Salicylic acid	1801042-01	2
EuRho	Salicylic acid	1901015-01	1
EuRho	Salicylic acid	1910018-01	1
EuRho	Salicylic acid	1910018-03	1
EuRho	Salicylic acid	2101028-01	1
euro AHD	Salicylic acid	1707009-025709	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Salicylic acid		1
Euro OTC	Salicylic acid	102455	1
Euro OTC	Salicylic acid	1110020	1
Euro OTC	Salicylic acid	1110020-01	4
Euro OTC	Salicylic acid	115465478596	1
Euro OTC	Salicylic acid	1206007-01	7
Euro OTC	Salicylic acid	130302001	1
Euro OTC	Salicylic acid	1303020-01	19
Euro OTC	Salicylic acid	1303020-02	4
Euro OTC	Salicylic acid	1406027-01	8
Euro OTC	Salicylic acid	140602702	1
Euro OTC	Salicylic acid	1406027-02	12
Euro OTC	Salicylic acid	1406027-02Mg1kg	1
Euro OTC	Salicylic acid	14076202	1
Euro OTC	Salicylic acid	1408027	1
Euro OTC	Salicylic acid	14E26-B04-294622	1
Euro OTC	Salicylic acid	1509007/02	1
Euro OTC	Salicylic acid	1509007-01	26
Euro OTC	Salicylic acid	150900702	1
Euro OTC	Salicylic acid	1509007-02	12
Euro OTC	Salicylic acid	1511023B	1
Euro OTC	Salicylic acid	15217301	1
Euro OTC	Salicylic acid	16/15-B08-330773	1
Euro OTC	Salicylic acid	16050013	1
Euro OTC	Salicylic acid	1605023/02	1
Euro OTC	Salicylic acid	160502301	2
Euro OTC	Salicylic acid	1605023-01	19
Euro OTC	Salicylic acid	160502302	1
Euro OTC	Salicylic acid	1605023-02	23
Euro OTC	Salicylic acid	160502331	1
Euro OTC	Salicylic acid	16E02-B09-325356	1
Euro OTC	Salicylic acid	1707009	1
Euro OTC	Salicylic acid	170700901	4
Euro OTC	Salicylic acid	1707009-01	26
Euro OTC	Salicylic acid	170700902	1
Euro OTC	Salicylic acid	1707009-02	14
Euro OTC	Salicylic acid	1707009-04	2
Euro OTC	Salicylic acid	1707009-1	1
Euro OTC	Salicylic acid	17133307	1
Euro OTC	Salicylic acid	17301509	1
Euro OTC	Salicylic acid	18001042-01	1
Euro OTC	Salicylic acid	1801042	1
Euro OTC	Salicylic acid	180104201	10
Euro OTC	Salicylic acid	1801042-01	54
Euro OTC	Salicylic acid	18050007	1
Euro OTC	Salicylic acid	19001501	1
Euro OTC	Salicylic acid	1901015-01	25
Euro OTC	Salicylic acid	1901015-02	14
Euro OTC	Salicylic acid	190101503	2
Euro OTC	Salicylic acid	1901015-03	12
Euro OTC	Salicylic acid	1901015-04	1
Euro OTC	Salicylic acid	1901018-03	1
Euro OTC	Salicylic acid	1910015-01	1
Euro OTC	Salicylic acid	191001801	2
Euro OTC	Salicylic acid	1910018-01	36
Euro OTC	Salicylic acid	1910018-02	9
Euro OTC	Salicylic acid	1910018-03	7
Euro OTC	Salicylic acid	1910018-18	1
Euro OTC	Salicylic acid	210102801	1
Euro OTC	Salicylic acid	2101028-01	18

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Salicylic acid	2108024-01	11
Euro OTC	Salicylic acid	2201044-01	2
Euro OTC	Salicylic acid	2201044-02	6
Euro OTC	Salicylic acid	2208003-01	2
Euro OTC	Salicylic acid	2208003-02	1
Euro OTC	Salicylic acid	ras1512800	1
Euro OTC	Salicylic acid	RAS1703500	2
Euro OTC	Salicylic acid	RAS1920400	1
Euro/Phönix	Salicylic acid	1801042-01	2
Euro	Salicylic acid	1509007-02	2
Europ Ots Pharma	Salicylic acid	12374205	1
EurRho/ Anzag	Salicylic acid	1509007-01	1
Fagaron	Salicylic acid	14Lo2-B02-303558	1
Fagron	Salicylic acid		2
Fagron	Salicylic acid	102455-0002	1
Fagron	Salicylic acid	11197121	1
Fagron	Salicylic acid	1140616	1
Fagron	Salicylic acid	11K10-N01	2
Fagron	Salicylic acid	11L19-N21	1
Fagron	Salicylic acid	12C20-N04	1
Fagron	Salicylic acid	12c20n12	1
Fagron	Salicylic acid	12C20-N12	5
Fagron	Salicylic acid	12H10-N03	8
Fagron	Salicylic acid	12H10-N08	3
Fagron	Salicylic acid	13344013	1
Fagron	Salicylic acid	13B14-N01	18
Fagron	Salicylic acid	13H01N01	1
Fagron	Salicylic acid	13H01-N01	6
Fagron	Salicylic acid	13H01N04	4
Fagron	Salicylic acid	13H01-N04	13
Fagron	Salicylic acid	13H01-N08	2
Fagron	Salicylic acid	13K08-B31-290852	5
Fagron	Salicylic acid	13K08-B31-290853	6
Fagron	Salicylic acid	14300801	1
Fagron	Salicylic acid	14300805	1
Fagron	Salicylic acid	14336920	1
Fagron	Salicylic acid	14B05B30	1
Fagron	Salicylic acid	14B05-B30	2
Fagron	Salicylic acid	14B05-B30-290854	5
Fagron	Salicylic acid	14E26_B04	1
Fagron	Salicylic acid	14E26B04	1
Fagron	Salicylic acid	14E26-B04	7
Fagron	Salicylic acid	14E26-B04_294623	1
Fagron	Salicylic acid	14E26-B04-294622	1
Fagron	Salicylic acid	14e26-b04-294623	1
Fagron	Salicylic acid	14e26-B04-294623	1
Fagron	Salicylic acid	14E26B04294623	1
Fagron	Salicylic acid	14E26-B04-294623	6
Fagron	Salicylic acid	14E26-B04-294624	7
Fagron	Salicylic acid	14E26-B04-296424	1
Fagron	Salicylic acid	14L02-B02	3
Fagron	Salicylic acid	14L02B02303557	1
Fagron	Salicylic acid	14L02-B02-303557	12
Fagron	Salicylic acid	14L02B02303558	1
Fagron	Salicylic acid	14L02-B02-303558	16
Fagron	Salicylic acid	15211806	2
Fagron	Salicylic acid	15211809	1
Fagron	Salicylic acid	16/15-B08-330773	3
Fagron	Salicylic acid	16/15-B08-331442	1
Fagron	Salicylic acid	16/15-B08-332098	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Salicylic acid	16/15-B08-333933	3
Fagron	Salicylic acid	1615-B08-330773	1
Fagron	Salicylic acid	1615B08332098	1
Fagron	Salicylic acid	16A18-B04	2
Fagron	Salicylic acid	16A18-B04322904	1
Fagron	Salicylic acid	16A18-B04-322904	3
Fagron	Salicylic acid	16A18-B04-322905	2
Fagron	Salicylic acid	16A18B04322905	2
Fagron	Salicylic acid	16E02-B09-325355	1
Fagron	Salicylic acid	16E02-B09-325356	2
Fagron	Salicylic acid	16I15-B08	1
Fagron	Salicylic acid	16I15-B08-327353	2
Fagron	Salicylic acid	16I15B08330773	1
Fagron	Salicylic acid	16I15-B08-330773	1
Fagron	Salicylic acid	16I15-B08-332098	1
Fagron	Salicylic acid	16I15-B08-333932	3
Fagron	Salicylic acid	17301502	1
Fagron	Salicylic acid	17C21B09	1
Fagron	Salicylic acid	17C21-B09	2
Fagron	Salicylic acid	17c21-b09-337172	1
Fagron	Salicylic acid	17C21-B09-337172	3
Fagron	Salicylic acid	17C21-B09-337173	4
Fagron	Salicylic acid	17c21-b09-337860	1
Fagron	Salicylic acid	17C21-B09-337860	3
Fagron	Salicylic acid	1801042-01	1
Fagron	Salicylic acid	18E24-B03	1
Fagron	Salicylic acid	18E24-B03-354310	3
Fagron	Salicylic acid	18E24-B03-354311	3
Fagron	Salicylic acid	18E24-B03-354312	1
Fagron	Salicylic acid	18F05-B02	2
Fagron	Salicylic acid	18F05-B02-350586	6
Fagron	Salicylic acid	18F05B02350587	2
Fagron	Salicylic acid	18F05-B02-350587	8
Fagron	Salicylic acid	18F05-B02-351974	3
Fagron	Salicylic acid	18F05-B02-352210	2
Fagron	Salicylic acid	18F05-B02-352528	1
Fagron	Salicylic acid	18F15-B02-350587	1
Fagron	Salicylic acid	1901015-03	1
Fagron	Salicylic acid	190262	1
Fagron	Salicylic acid	190263	20
Fagron	Salicylic acid	190263RAS1818100	1
Fagron	Salicylic acid	190264	15
Fagron	Salicylic acid	19B12-B04	2
Fagron	Salicylic acid	19B12-B04-193458	1
Fagron	Salicylic acid	19B12-B04-193459	2
Fagron	Salicylic acid	19B12-B04-193460	7
Fagron	Salicylic acid	20A29-B31	1
Fagron	Salicylic acid	20A29-B31-197697	6
Fagron	Salicylic acid	20E21-B03	5
Fagron	Salicylic acid	20e21-B03-200496	1
Fagron	Salicylic acid	20E21B03200496	1
Fagron	Salicylic acid	20E21-B03-200496	8
Fagron	Salicylic acid	20E21-Bo3-200496	1
Fagron	Salicylic acid	20E21-BO3-200496	1
Fagron	Salicylic acid	20E32-B03-200496	1
Fagron	Salicylic acid	20G20-B04	1
Fagron	Salicylic acid	20G20-B04-202192	3
Fagron	Salicylic acid	20G20-B04-202193	1
Fagron	Salicylic acid	21003008004	1
Fagron	Salicylic acid	21A26-B19-210110	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Salicylic acid	21a26-b19-210141	1
Fagron	Salicylic acid	21A26-B19-210141	3
Fagron	Salicylic acid	21G21-B04-217748	1
Fagron	Salicylic acid	21G30B03215511	1
Fagron	Salicylic acid	21G30-B03-215511	6
Fagron	Salicylic acid	21G3O-BO3-2155101	1
Fagron	Salicylic acid	21J06B11-217750	1
Fagron	Salicylic acid	21J06-B11-217750	2
Fagron	Salicylic acid	2201115	1
Fagron	Salicylic acid	22E12-B05-224210	1
Fagron	Salicylic acid	290852	1
Fagron	Salicylic acid	3111Q-01045	1
Fagron	Salicylic acid	AS28012021	1
Fagron	Salicylic acid	B03-2004906	2
Fagron	Salicylic acid	B19-210110	1
Fagron	Salicylic acid	B31-1976907	3
Fagron	Salicylic acid	RAS1135100	1
Fagron	Salicylic acid	RAS1135300	1
Fagron	Salicylic acid	RAS1808500	1
Fagron	Salicylic acid	RAS1818100	4
Fagron	Salicylic acid	RAS1929500	1
Fagron	Salicylic acid	xxxxxxxx	1
Fargon / AHD	Salicylic acid	20E21-B03-200496	2
Fargon	Salicylic acid	14L02-B02	1
Farmalabor / Farmalabor	Salicylic acid	P1404195-002	1
Fiebig/Maros	Salicylic acid	1707009-02	1
Fiebig	Salicylic acid	15211810	1
Fiebig	Salicylic acid	16010905	1
Fiebig	Salicylic acid	17301506	1
Fiebig	Salicylic acid	17301509	1
Fiebig	Salicylic acid	18147321	1
Gatt-Koller	Salicylic acid	1803840	2
Gehe / Spinnrad	Salicylic acid	16050005	1
Gehe amax	Salicylic acid	12036223	1
Gehe amax	Salicylic acid	1801042-01	1
Gehe amax	Salicylic acid	18147302	1
Gehe amax	Salicylic acid	18147314	1
Gehe/ Caesar & Loret…	Salicylic acid	20000146005	1
Gehe	Salicylic acid		1
Gehe	Salicylic acid	1050313	1
Gehe	Salicylic acid	11D15-N08	1
Gehe	Salicylic acid	1206007-01	1
Gehe	Salicylic acid	13B14-N01	1
Gehe	Salicylic acid	13H01-N04	1
Gehe	Salicylic acid	14336919	1
Gehe	Salicylic acid	14E26-B04-294624	1
Gehe	Salicylic acid	14L02-B02-303558	1
Gehe	Salicylic acid	15217301	1
Gehe	Salicylic acid	15217304	1
Gehe	Salicylic acid	16010910	1
Gehe	Salicylic acid	16050013	1
GEHE	Salicylic acid	1605023-01	1
GEHE	Salicylic acid	1605023-02	2
Gehe	Salicylic acid	16312003	1
Gehe	Salicylic acid	165023-02	1
gehe	Salicylic acid	16I15-B08-331442	1
Gehe	Salicylic acid	1707009-01	1
GEHE	Salicylic acid	1707009-01	1
GEHE	Salicylic acid	1707009-02	1
Gehe	Salicylic acid	17133301	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Salicylic acid	17133307	4
GEHE	Salicylic acid	17301502	2
Gehe	Salicylic acid	17301511	1
GEHE	Salicylic acid	17301511	1
Gehe	Salicylic acid	17C21-B09-337172	1
Gehe	Salicylic acid	18147314	1
GEHE	Salicylic acid	18147317	1
Gehe	Salicylic acid	18147321	1
Gehe	Salicylic acid	18230007	1
GEHE	Salicylic acid	18230009	1
Gehe	Salicylic acid	18F05-B02-350586	1
Gehe	Salicylic acid	20000147002	1
Gehe	Salicylic acid	20000147004	1
Gehe	Salicylic acid	20000147006	2
Gehe	Salicylic acid	20003823008	2
Gehe	Salicylic acid	2000442010	2
Gehe	Salicylic acid	20004424015	1
Gehe	Salicylic acid	21003008010	1
Gehe	Salicylic acid	21003008016	1
GEHE	Salicylic acid	22001529002	1
gehe	Salicylic acid	22003107004	1
Gehe	Salicylic acid	2208003-01	1
Gehe	Salicylic acid	2208003-02	1
Gehe	Salicylic acid	22D07-B03-221811	2
gehe	Salicylic acid	2308012-01	1
Gehe	Salicylic acid	2308012-01	1
Gehe	Salicylic acid	24000043001	1
Geibo 5.7.21	Salicylic acid	20A29-B31-197697	1
Geilenkirchen	Salicylic acid	17301506	1
Geilenkirchen	Salicylic acid	192209001	2
Gutenberg-Apotheke	Salicylic acid	12374208	1
Hänseler	Salicylic acid		7
Hofmann & Sommer	Salicylic acid	1230	3
Holdermann	Salicylic acid	14E26-B04294624	1
Ichthyol/ Noweda	Salicylic acid	17133303	1
Ichthyol/Noweda	Salicylic acid	13344003	1
Jenne	Salicylic acid	12345	1
Jenne	Salicylic acid	18147314	1
Jenne	Salicylic acid	20000147004	1
Jenne	Salicylic acid	20003823016	2
Jenne	Salicylic acid	22J26B06-227888	1
Kehr	Salicylic acid	16312001	2
Kehr	Salicylic acid	16312012	1
Kehr	Salicylic acid	17301509	1
Kehr	Salicylic acid	2201044-02	1
Kehr	Salicylic acid	23003599002	1
Klenk	Salicylic acid	12134722	1
Krieger	Salicylic acid	13032017-MW-A	1
Krieger	Salicylic acid	16050012	1
L30	Salicylic acid	16312005	1
L30	Salicylic acid	17301505	1
L30	Salicylic acid	17301507	1
Midas	Salicylic acid	16312010	1
Novacyl / Ebert	Salicylic acid	14336911	2
Novacyl / Ebert	Salicylic acid	14336919	1
Novacyl / Gehe	Salicylic acid	16010912	1
Novacyl / Gehe	Salicylic acid	18147321	1
Novacyl, FR	Salicylic acid	15084403	2
Novacyl/Caesar & Lor…	Salicylic acid	17301505	1
Novacyl/Gehe Pharma …	Salicylic acid	17301507	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Novacyl/Phoenix	Salicylic acid	RAS1817400	1
Novacyl/Phoenix	Salicylic acid	RAS1818100	2
Novacyl/Phoenix	Salicylic acid	RAS1907500	1
Novacyl	Salicylic acid	1707009-02	1
Novacyl	Salicylic acid	1910018-01	1
Novacyl	Salicylic acid	RAS1821600	1
Noweda/ Caesar&Loren…	Salicylic acid	192209001	1
Noweda/ Infecto Pharm	Salicylic acid	16/15-08-330773	1
Noweda/Fargon	Salicylic acid	14L02-B02-303556	1
Noweda	Salicylic acid	12036215	1
Noweda	Salicylic acid	12036226	1
Noweda	Salicylic acid	1406027-01	1
Noweda	Salicylic acid	140602702	1
Noweda	Salicylic acid	14336907	2
Noweda	Salicylic acid	16/15-B08-330773	1
Noweda	Salicylic acid	16050011	1
Noweda	Salicylic acid	16050013	1
Noweda	Salicylic acid	1707009-02	2
Noweda	Salicylic acid	170700904	3
Noweda	Salicylic acid	17133304	1
noweda	Salicylic acid	17301502	1
Noweda	Salicylic acid	17304506	1
Noweda	Salicylic acid	180104201	1
Noweda	Salicylic acid	181473001	2
Noweda	Salicylic acid	1901015	1
Noweda	Salicylic acid	1901015-01	1
Noweda	Salicylic acid	1901015-03	1
Noweda	Salicylic acid	190263	1
Noweda	Salicylic acid	19061206	1
Noweda	Salicylic acid	19B12-B04-193459	1
Noweda	Salicylic acid	20003823008	1
noweda	Salicylic acid	20004424015	1
Noweda	Salicylic acid	210802401	1
Noweda	Salicylic acid	22001524003	1
Noweda	Salicylic acid	22001528002	1
Noweda	Salicylic acid	22001528003	2
Noweda	Salicylic acid	22001529002	1
noweda	Salicylic acid	22001534003	1
Noweda	Salicylic acid	2208003_01	1
Noweda	Salicylic acid	2208003-02	1
Noweda	Salicylic acid	AS10052021	1
Noweda	Salicylic acid	P2021/113	1
Phoenix 09.10.2017	Salicylic acid	16050017	1
Phoenix goettingen	Salicylic acid	14300808	1
Phoenix/Cealo	Salicylic acid	1733303	1
Phoenix/Cealo	Salicylic acid	3414M-01045	1
Phoenix	Salicylic acid	12H10-No8	1
Phoenix	Salicylic acid	14076201	1
Phoenix	Salicylic acid	15211808	2
Phoenix	Salicylic acid	16050012	1
Phoenix	Salicylic acid	16312005	1
Phoenix	Salicylic acid	17301502	1
Phoenix	Salicylic acid	18050007	1
Phoenix	Salicylic acid	18147308	1
Phoenix	Salicylic acid	19061202	1
Phoenix	Salicylic acid	1910018-02	1
Phoenix	Salicylic acid	191411012	1
Phoenix	Salicylic acid	20004424006	1
Phoenix	Salicylic acid	20004424007	1
Phoenix	Salicylic acid	22001529002	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Salicylic acid	22001534003	2
Phoenix	Salicylic acid	2208003-01	1
Phoenox	Salicylic acid	20000147004	1
Phönix 02.08.2019	Salicylic acid	18230009	1
Phönix Gotha	Salicylic acid	12374207	1
Phönix Gotha	Salicylic acid	14076201	1
Phönix Gotha	Salicylic acid	14300801	1
Phönix Gotha	Salicylic acid	18050006	1
Phönix	Salicylic acid	11311917	1
Phönix	Salicylic acid	12323401	1
Phönix	Salicylic acid	12374210	1
Phönix	Salicylic acid	12374211	1
Phönix	Salicylic acid	12C20-N12	1
Phönix	Salicylic acid	1303020-01	3
Phönix	Salicylic acid	13K08-B31-290853	1
Phönix	Salicylic acid	1509007-02	1
Phönix	Salicylic acid	16050005	1
Phönix	Salicylic acid	16050012	1
Phönix	Salicylic acid	16a18-b04-322905	1
Phönix	Salicylic acid	1713303	1
Phönix	Salicylic acid	17301506	1
Phönix	Salicylic acid	17301507	1
Phonix	Salicylic acid	18050007	1
Phönix	Salicylic acid	18050009	5
Phönix	Salicylic acid	18147302	1
Phönix	Salicylic acid	18147303	2
Phönix	Salicylic acid	18147314	2
Phönix	Salicylic acid	190612001	1
Phönix	Salicylic acid	200004424001	1
phönix	Salicylic acid	20004424004	1
Phönix	Salicylic acid	20004424004	1
Phönix	Salicylic acid	20004424006	1
Phönix	Salicylic acid	2101028-01	1
Phönix	Salicylic acid	2108024-01	2
Phönix	Salicylic acid	22001529002	2
Phönix	Salicylic acid	22001534003	1
Phönix	Salicylic acid	3177	1
Phönix	Salicylic acid	68/AKD4	1
Röntgen	Salicylic acid	190612004	1
Salicylsäure	Salicylic acid	190612001	1
Sana 04.02.17 Ek:13,83	Salicylic acid	16010910	1
Sanacorp 28.01.15 EK…	Salicylic acid	14076204	1
Sanacorp	Salicylic acid	11311922	1
Sanacorp	Salicylic acid	12134707	1
Sanacorp	Salicylic acid	12134712	1
Sanacorp	Salicylic acid	12134715	1
Sanacorp	Salicylic acid	123036223	1
Sanacorp	Salicylic acid	12374205	1
Sanacorp	Salicylic acid	12374210	1
Sanacorp	Salicylic acid	1303020-01	1
Sanacorp	Salicylic acid	13344014	1
Sanacorp	Salicylic acid	13344018	1
Sanacorp	Salicylic acid	15084404	1
Sanacorp	Salicylic acid	16010910	1
Sanacorp	Salicylic acid	16010912	1
Sanacorp	Salicylic acid	16050005	1
Sanacorp	Salicylic acid	16050012	1
Sanacorp	Salicylic acid	17133307	1
Sanacorp	Salicylic acid	171333307	1
Sanacorp	Salicylic acid	17301505	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Salicylic acid	17301506	1
Sanacorp	Salicylic acid	17301509	1
Sanacorp	Salicylic acid	17C21-B09-339446	1
Sanacorp	Salicylic acid	18050006	1
Sanacorp	Salicylic acid	18050007	1
Sanacorp	Salicylic acid	18147303	1
Sanacorp	Salicylic acid	1910018-03	1
Sanacorp	Salicylic acid	20000147002	1
Sanacorp	Salicylic acid	2000442406	1
Sanacorp	Salicylic acid	20E21-B03-200496	1
Sanacorp	Salicylic acid	2101028-01	1
Sanacorp	Salicylic acid	21A26-B19-210110	1
sanacorp	Salicylic acid	22001528002	1
Sanacorp	Salicylic acid	22001529002	1
Sanacorp	Salicylic acid	22001534003	1
Sanacorp	Salicylic acid	23002014003	1
Sanacorp	Salicylic acid	68/AKD2	1
Spangropharm	Salicylic acid	11197104	1
VDL	Salicylic acid	11197122	1
VDL	Salicylic acid	22D07-B03-221811	1
xxx	Salicylic acid	4311A-01045	1

- 231 760 spectra from 1515 *Apo-Ident* customers from a total of 48 672 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Salicylic acid* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Salicylic acid* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	460	0	152 502
Type B	0	1120	0	200 964
Type C	0	4283	24	231 760

The substance/substance group *Salicylic acid* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6957 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.4643 %)
Type C	100.0000 % (> 99.9007 %)	99.4428 % (> 99.3731 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20696	21906	6.53	218.15
21436	21906	6.44	218.53
21760	21906	2.74	221.03
21906	21906	0.00	221.18
22443	22443	0.00	210.55
23592	21906	3.47	222.12
24591	21906	4.97	222.14
25543	25543	0.00	220.90
26113	26113	0.00	213.34

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Selenium yeast**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20906-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Selenium yeast

Special notes

When selecting the *Selenium yeast* substance/substance group, the following information is displayed to the user:

- Advice: Currently no longer available from major pharmaceutical manufacturers. Therefore, batch maintenance is currently not possible.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Selenium yeast	5	2	5

Second-stage model

For differentiation of the substance/substance group *Selenium yeast* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Selenium yeast* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	31.31	25.15
Riboflavin sodium phosphate hydrate	69.20	–
⋮	⋮	⋮
Colistin sulfate	>50	20.97
Bacitracin	>50	26.14
Amphotericin B	>50	27.65
Nystatin	>50	37.22
Riboflavin	>50	47.43
Estradiol hemihydrate	>50	52.52
Calcium glycerophosphate	>50	53.68
Carmellose sodium	>50	61.49
Calcium pantothenate	>50	62.24
Cyanocobalamin	>50	71.20
alpha-tocopheryl acetate dry concentrate	>50	82.54
Gelatine, white	>50	83.31
Estriol	>50	92.50
SyrSpend® SF Alka	>50	93.75
Triamcinolone	>50	105.76
Methylcobalamin	>50	132.15
Tosylchloramide sodium	>50	136.53
Rice starch	>50	140.36
Hyoscine hydrobromide	>50	143.68
SyrSpend® SF pH4 neo (Maize starch)	>50	164.42
Corn starch	>50	174.47
Acacia, dried dispersion	>50	194.84
Oxalic acid	>50	228.71
Maltodextrin	>50	252.81
Wheat starch	>50	256.85
SyrSpend® SF pH4	>50	260.47
Potato starch	>50	297.40
Fructose	>50	395.94

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Selenium yeast* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Selenium yeast*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Selenium yeast	13347911	21377	40	1509355
Caelo	Selenium yeast	17002202	23120	40	1707512
Caelo	Selenium yeast	17002208	23446	40	20170126
Caelo	Selenium yeast	173332	24038	40	20180207*
Caelo	Selenium yeast	192450005	25522	40	2106135

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 5 reference samples from the substance/substance group *Selenium yeast*. These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.
- 152 762 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 3 reference samples from the substance/substance group *Selenium yeast*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Selenium yeast	20003859005	25979	40
Euro OTC	Selenium yeast	L1401013-01	21102	40
Caelo	Selenium yeast	20003859005	25979SI	10

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 994 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 3 *Apo-Ident* customers from 6 batches from the substance/substance group *Selenium yeast*.
- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Selenium yeast	13347906	1
Caelo	Selenium yeast	13347911	1
Caelo	Selenium yeast	15276208	1
Caesar & Loretz GmbH...	Selenium yeast	11318111	1
Euro OTC	Selenium yeast	L1910012-01	1
Euro OTC	Selenium yeast	L1910012-1	1

- 236 061 spectra from 1515 *Apo-Ident* customers from a total of 49 252 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Selenium yeast* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Selenium yeast* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	90	0	201 994
Type C	0	5	1	236 060

The substance/substance group *Selenium yeast* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 93.3333 %)
Type C	100.0000 % (> 99.9020 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21377	21377	0.00	78.05
23120	23120	0.00	65.96
23446	23120	5.21	63.32
24038	24038	0.00	70.75
25522	25522	0.00	72.73

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Serine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	22289-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Serine; L-serine; Serinum

Special notes

When selecting the *Serine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Serine	8	8	3

Second-stage model

For differentiation of the substance/substance group *Serine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Serine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	81.75	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Serine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Serine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Serine	1512012	22289	60	20160112*
Euro OTC	Serine	1606020-01	22668	40	20160714
Euro OTC	Serine	1606020	22678	40	20160714*
Euro OTC	Serine	1711033	23914	40	20171208*
Euro OTC	Serine	1904034	24641	40	20190521*
Euro OTC	Serine	1909027	24956	40	20191015*
Euro OTC	Serine	2011007	25471	40	20201127*
Fagron	Serine	21J20-B02-216460	26156	40	20220114
Fagron	Serine	21J20-B02-216460	26156SI	20	20220114

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Serine*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 602 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 370 spectra of 10 reference samples from the substance/substance group *Serine*.
- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Serine	1611006	22922	40
Euro OTC	Serine	1809016	24296	40
Euro OTC	Serine	2006028	25305	40
Euro OTC	Serine	2107017	25776	50
Euro OTC	Serine	2206022	26275	40
Euro OTC	Serine	2302004	26599	40
Euro OTC	Serine	2308017	27206	40
Fagron	Serine	23J09-B02-235857	27049	40
Euro OTC	Serine	2206022	26275SI	20
Euro OTC	Serine	2302004	26599SI	20

- 201 714 spectra from a total of 4037 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6 spectra from 2 *Apo-Ident* customers from 4 batches from the substance/substance group *Serine*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Serine	1606020-01	3
Euro OTC	Serine	1904034-01	1
Euro OTC	Serine	2006028-01	1
Euro OTC	Serine	2206022-01	1

- 236 061 spectra from 1515 *Apo-Ident* customers from a total of 49 254 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Serine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Serine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	370	0	201 714
Type C	0	6	0	236 061

The substance/substance group *Serine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.3784 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22289	22289	0.00	202.35
22668	22678	6.14	208.56
22678	22678	0.00	208.53
23914	23914	0.00	206.60
24641	24641	0.00	209.24
24956	24956	0.00	203.40
25471	25471	0.00	208.75
26156	23914	15.51	208.15

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sildenafil citrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20852-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sildenafil citrate; Sildenafili citras

Special notes

When selecting the *Sildenafil citrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sildenafil citrate	7	10	197

Second-stage model

For differentiation of the substance/substance group *Sildenafil citrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sildenafil citrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	101.23	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sildenafil citrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sildenafil citrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sildenafil citrate	160498	22446	60	20160307*
Caelo	Sildenafil citrate	170715	23336	40	20170529*
Caelo	Sildenafil citrate	170715	23345	40	20170529*
Euro OTC	Sildenafil citrate	1311010-01	21621	60	20131209
Euro OTC	Sildenafil citrate	1311010-04	23178	40	20150309
Euro OTC	Sildenafil citrate	1908006	24843	40	20190906*
Fagron	Sildenafil citrate	13F24-N03	20852	40	1402052
Fagron	Sildenafil citrate	13J15-N01	20927	80	20131030

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 400 spectra of 8 reference samples from the substance/substance group *Sildenafil citrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 562 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 540 spectra of 14 reference samples from the substance/substance group *Sildenafil citrate*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sildenafil citrate	190866	24545	40
Caelo	Sildenafil citrate	22000907	26248	40
Caelo	Sildenafil citrate	23003271	27247	40
Euro OTC	Sildenafil citrate	1807037	24192	40
Euro OTC	Sildenafil citrate	1902031	24469	40
Euro OTC	Sildenafil citrate	2003003	25380	40
Euro OTC	Sildenafil citrate	2111002	25896	50
Euro OTC	Sildenafil citrate	2301014	26580	40
Euro OTC	Sildenafil citrate	2403010	27287	40
Fagron	Sildenafil citrate	21G10-B25-219206	26072	40
Caelo	Sildenafil citrate	22000907	26248SI	20
Euro OTC	Sildenafil citrate	2111002	25896SI	50
Euro OTC	Sildenafil citrate	2301014	26580SI	20
Fagron	Sildenafil citrate	21G10-B25-219206	26072SI	40

- 201 544 spectra from a total of 4035 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 743 spectra from 178 *Apo-Ident* customers from 206 batches from the substance/substance group *Sildenafil citrate*.

- Among them are spectra of independent samples from 196 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sildenafil citrate	1311010-04	2
	Sildenafil citrate	2111002-01	1
	Sildenafil citrate	22000907002	2
	Sildenafil citrate	22000907012	2
	Sildenafil citrate	22000907015	5
	Sildenafil citrate	22000907016	3
	Sildenafil citrate	22000907018	3
	Sildenafil citrate	23000811001	5
	Sildenafil citrate	23000811003	2
	Sildenafil citrate	23003271003	2
	Sildenafil citrate	2301014-01	5
	Sildenafil citrate	23L11-B05-236845	1
	Sildenafil citrate	7-22792004	1
	Sildenafil citrate	B07-2279203	1
	Sildenafil citrate	SLC/0221061	1
	Sildenafil citrate	SLC/1123066	1
AHC	Sildenafil citrate	21B17-B09-203496	2
AHC	Sildenafil citrate	23003271003	1
AHC	Sildenafil citrate	2301014-01	1
Alliance	Sildenafil citrate		1
Alliance	Sildenafil citrate	1311010-03	1
Caelo	Sildenafil citrate		1
Caelo	Sildenafil citrate	101051528	1
Caelo	Sildenafil citrate	1311010-06	1
Caelo	Sildenafil citrate	14074703	2
Caelo	Sildenafil citrate	14074707	2
Caelo	Sildenafil citrate	14074709	1
Caelo	Sildenafil citrate	14074714	5
Caelo	Sildenafil citrate	14074715	5
Caelo	Sildenafil citrate	14074716	1
Caelo	Sildenafil citrate	1407474	1
Caelo	Sildenafil citrate	15097301	1
Caelo	Sildenafil citrate	15097302	1
Caelo	Sildenafil citrate	15097303	1
Caelo	Sildenafil citrate	15097306	1
Caelo	Sildenafil citrate	15097307	2
Caelo	Sildenafil citrate	15097308	1
Caelo	Sildenafil citrate	15097310	3
Caelo	Sildenafil citrate	15097311	1
Caelo	Sildenafil citrate	15097312	2
Caelo	Sildenafil citrate	15097315	1
Caelo	Sildenafil citrate	15097317	2
Caelo	Sildenafil citrate	15F11-B02-309081	1
Caelo	Sildenafil citrate	15F11-B02-314725	1
Caelo	Sildenafil citrate	16049801	1
Caelo	Sildenafil citrate	16049802	10
Caelo	Sildenafil citrate	16049805	1
Caelo	Sildenafil citrate	16049808	4
Caelo	Sildenafil citrate	16049810	2
Caelo	Sildenafil citrate	16049811	1
Caelo	Sildenafil citrate	16049812	1
Caelo	Sildenafil citrate	16049814	9
Caelo	Sildenafil citrate	16049819	1
Caelo	Sildenafil citrate	16049820	5
Caelo	Sildenafil citrate	16049821	13
Caelo	Sildenafil citrate	16049823	2
Caelo	Sildenafil citrate	16049824	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sildenafil citrate	16049826	1
Caelo	Sildenafil citrate	16F30-B02-3241715	1
Caelo	Sildenafil citrate	17071502	2
Caelo	Sildenafil citrate	17071503	7
Caelo	Sildenafil citrate	17071504	21
Caelo	Sildenafil citrate	17344001	2
Caelo	Sildenafil citrate	17344003	11
Caelo	Sildenafil citrate	17344004	2
Caelo	Sildenafil citrate	17344005	9
Caelo	Sildenafil citrate	17344006	2
Caelo	Sildenafil citrate	17344008	4
Caelo	Sildenafil citrate	17344009	3
Caelo	Sildenafil citrate	1734401	1
Caelo	Sildenafil citrate	17344010	2
Caelo	Sildenafil citrate	17344014	3
Caelo	Sildenafil citrate	17344015	1
Caelo	Sildenafil citrate	18B13-B06-349160	2
Caelo	Sildenafil citrate	18B13-B06-351981	1
Caelo	Sildenafil citrate	1908006-01	2
Caelo	Sildenafil citrate	1908006-02	1
Caelo	Sildenafil citrate	190866001	2
Caelo	Sildenafil citrate	190866005	2
Caelo	Sildenafil citrate	19086603	3
Caelo	Sildenafil citrate	19086604	8
Caelo	Sildenafil citrate	19086605	12
Caelo	Sildenafil citrate	19086605P-191112-1	1
Caelo	Sildenafil citrate	19086605P-191212-1	1
Caelo	Sildenafil citrate	19086605P-200107-1	1
Caelo	Sildenafil citrate	19086605P-200206-2	1
Caelo	Sildenafil citrate	19086606	10
Caelo	Sildenafil citrate	19086606P-200319-5	1
Caelo	Sildenafil citrate	19086607	2
Caelo	Sildenafil citrate	190866606	1
Caelo	Sildenafil citrate	2000016003	1
Caelo	Sildenafil citrate	20000163002	9
Caelo	Sildenafil citrate	20000163002/01	1
Caelo	Sildenafil citrate	20000163003	5
Caelo	Sildenafil citrate	20000163005	1
Caelo	Sildenafil citrate	20000163006	3
Caelo	Sildenafil citrate	2000163003	2
Caelo	Sildenafil citrate	20004485002	2
Caelo	Sildenafil citrate	20004485003	7
Caelo	Sildenafil citrate	21000810001	6
Caelo	Sildenafil citrate	21000810002	2
Caelo	Sildenafil citrate	21000810003	6
Caelo	Sildenafil citrate	21000810004	3
Caelo	Sildenafil citrate	21000810006	2
Caelo	Sildenafil citrate	21000810008	3
Caelo	Sildenafil citrate	21000810010	4
Caelo	Sildenafil citrate	21000810011	2
Caelo	Sildenafil citrate	21000810012	1
Caelo	Sildenafil citrate	2100081008	1
Caelo	Sildenafil citrate	2100810006	1
Caelo	Sildenafil citrate	2101403	1
Caelo	Sildenafil citrate	22000907001	3
Caelo	Sildenafil citrate	22000907002	6
Caelo	Sildenafil citrate	22000907008	1
Caelo	Sildenafil citrate	22000907012	1
Caelo	Sildenafil citrate	2200090907015	1
Caelo	Sildenafil citrate	2200907002	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sildenafil citrate	46049826	1
Caelo	Sildenafil citrate	SLC/0420004	1
Caesar & Loretz GmbH...	Sildenafil citrate	21000810008	1
Caesar & Loretz GmbH...	Sildenafil citrate	22000907002	2
Caesar & Loretz GmbH...	Sildenafil citrate	20004485003	1
Caesar & Loretz GmbH/Gehe	Sildenafil citrate	19086607	3
Caesar & Loretz GmbH...	Sildenafil citrate	190866001	2
Caesar & Loretz GmbH...	Sildenafil citrate	20000163003	2
Caesar & Loretz GmbH...	Sildenafil citrate	21000810008	1
Caesar & Loretz GmbH...	Sildenafil citrate	21000810013	1
Caesar & Loretz GmbH...	Sildenafil citrate	21000810003	1
Caesar & Loretz GmbH...	Sildenafil citrate	190866003	1
Caesar & Loretz GmbH...	Sildenafil citrate	20000163004	6
Caesar & Loretz GmbH/Sana	Sildenafil citrate	19086604	1
Caesar & Loretz GmbH...	Sildenafil citrate	21000810006	1
Caesar & Loretz GmbH...	Sildenafil citrate	21000810011	1
Caesar & Loretz GmbH...	Sildenafil citrate	22000907002	1
Caesar & Loretz GmbH	Sildenafil citrate	17344013	1
Caesar & Loretz GmbH	Sildenafil citrate	17344014	1
Caesar & Loretz GmbH	Sildenafil citrate	180737-01	1
Caesar & Loretz GmbH	Sildenafil citrate	190866005	1
Caesar & Loretz GmbH	Sildenafil citrate	19086601	1
Caesar & Loretz GmbH	Sildenafil citrate	19086603	1
Caesar & Loretz GmbH	Sildenafil citrate	19086605	1
Caesar & Loretz GmbH	Sildenafil citrate	19086606	10
Caesar & Loretz GmbH	Sildenafil citrate	19086607	2
Caesar & Loretz GmbH	Sildenafil citrate	20000163002	3
Caesar & Loretz GmbH	Sildenafil citrate	20004485003	3
Caesar & Loretz GmbH	Sildenafil citrate	21000810003	7
Caesar & Loretz GmbH	Sildenafil citrate	21000810004	1
Caesar & Loretz GmbH	Sildenafil citrate	21000810006	5
Caesar & Loretz GmbH	Sildenafil citrate	21000810007	1
Caesar & Loretz GmbH	Sildenafil citrate	21000810008	1
Caesar & Loretz GmbH	Sildenafil citrate	21000810011	1
Caesar & Loretz GmbH	Sildenafil citrate	21000810012	4
Caesar & Loretz GmbH	Sildenafil citrate	21000810013	2
Caesar & Loretz GmbH	Sildenafil citrate	21000810014	2
Caesar & Loretz GmbH	Sildenafil citrate	2100081003	1
Caesar & Loretz GmbH	Sildenafil citrate	22000907001	6
Caesar & Loretz GmbH	Sildenafil citrate	22000907002	4
Caesar & Loretz GmbH	Sildenafil citrate	22000907012	2
Caesar & Loretz GmbH	Sildenafil citrate	22000907013	2
Caesar & Loretz GmbH	Sildenafil citrate	22000907018	1
Caesar & Loretz GmbH	Sildenafil citrate	B01-2018201	1
Cealo	Sildenafil citrate	16049805	1
Cealo	Sildenafil citrate	20000163005	1
Eu Rho	Sildenafil citrate	1902031-01	1
Eu Rho	Sildenafil citrate	1908006-01	1
EuRho/Noweda	Sildenafil citrate	1807037-01	3
EuRho	Sildenafil citrate	2111002-01	2
Euro OTC	Sildenafil citrate		1
Euro OTC	Sildenafil citrate	10061706	1
Euro OTC	Sildenafil citrate	101031827	1
Euro OTC	Sildenafil citrate	103031328	1
Euro OTC	Sildenafil citrate	13110-01	1
Euro OTC	Sildenafil citrate	1311010	1
Euro OTC	Sildenafil citrate	1311010-01	4
Euro OTC	Sildenafil citrate	1311010-02	2
Euro OTC	Sildenafil citrate	131101003	1
Euro OTC	Sildenafil citrate	1311010-03	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Sildenafil citrate	131101004	1
Euro OTC	Sildenafil citrate	1311010-04	3
Euro OTC	Sildenafil citrate	1311010-05	6
Euro OTC	Sildenafil citrate	1311010-06	11
Euro OTC	Sildenafil citrate	1311010-07	1
Euro OTC	Sildenafil citrate	1311010-6	1
Euro OTC	Sildenafil citrate	14051402	1
Euro OTC	Sildenafil citrate	15081830	1
Euro OTC	Sildenafil citrate	15097301	1
Euro OTC	Sildenafil citrate	17061405	1
Euro OTC	Sildenafil citrate	17081504	1
Euro OTC	Sildenafil citrate	1807037-01	19
Euro OTC	Sildenafil citrate	1807037-01x2	1
Euro OTC	Sildenafil citrate	19011907	1
Euro OTC	Sildenafil citrate	1902031-01	30
Euro OTC	Sildenafil citrate	19080006-01	1
Euro OTC	Sildenafil citrate	1908006-01	22
Euro OTC	Sildenafil citrate	1908006-02	9
Euro OTC	Sildenafil citrate	19b07-b02-191473	1
Euro OTC	Sildenafil citrate	2003003-01	17
Euro OTC	Sildenafil citrate	2003003-02	12
Euro OTC	Sildenafil citrate	2111002-01	19
Euro OTC	Sildenafil citrate	2111002-1	1
Euro OTC	Sildenafil citrate	2301014-01	2
Euro OTC	Sildenafil citrate	27021802	1
Euro OTC	Sildenafil citrate	311010-06	1
Euro OTC	Sildenafil citrate	5117Q-03684	1
Euro	Sildenafil citrate	1311010-06	1
Euro	Sildenafil citrate	190020031-01	1
euro	Sildenafil citrate	1908006-01	2
Fagron	Sildenafil citrate	13J15-N01	2
Fagron	Sildenafil citrate	14H11-B01-303183	1
Fagron	Sildenafil citrate	15F11-B02	2
Fagron	Sildenafil citrate	15F11-B02-314725	1
Fagron	Sildenafil citrate	15f11-b02-320186	1
Fagron	Sildenafil citrate	15F11-B02-320186	1
Fagron	Sildenafil citrate	15F11-B02-525175	3
Fagron	Sildenafil citrate	16049812	1
Fagron	Sildenafil citrate	16049817	1
Fagron	Sildenafil citrate	16049819	2
Fagron	Sildenafil citrate	16A18-B08	2
Fagron	Sildenafil citrate	16F30-B02	1
Fagron	Sildenafil citrate	16F30-B02-324715	3
Fagron	Sildenafil citrate	16F30-B02-331449	1
Fagron	Sildenafil citrate	16F30-B02-331450	4
Fagron	Sildenafil citrate	16F30-B02-334977	2
Fagron	Sildenafil citrate	16F30-BO2-324715	1
Fagron	Sildenafil citrate	17071505	1
Fagron	Sildenafil citrate	17H31-B02-342459	4
Fagron	Sildenafil citrate	18B13-B06	1
Fagron	Sildenafil citrate	18B13-B06-347389	2
Fagron	Sildenafil citrate	18B13-B06-348000	1
Fagron	Sildenafil citrate	18B13-B06-348001	2
Fagron	Sildenafil citrate	18B13-B06-349160	2
Fagron	Sildenafil citrate	18B13-B06-351981	1
Fagron	Sildenafil citrate	18B13-B06-353827	1
Fagron	Sildenafil citrate	19807-B02-194729	1
Fagron	Sildenafil citrate	19807-B02-194730	1
Fagron	Sildenafil citrate	19B07-802-194730	1
Fagron	Sildenafil citrate	19B07-B02-191472	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Sildenafil citrate	19B07-B02-191473	4
Fagron	Sildenafil citrate	19B07-B02-191474	1
Fagron	Sildenafil citrate	19B07-B02-194728	2
Fagron	Sildenafil citrate	19B07-B02-194729	2
Fagron	Sildenafil citrate	19K12-B01-195593	1
Fagron	Sildenafil citrate	19K12-B01-195594	6
Fagron	Sildenafil citrate	19K12-BO1-195594	1
Fagron	Sildenafil citrate	19K12-BO1-195595	1
Fagron	Sildenafil citrate	20J26-B01-201822	7
Fagron	Sildenafil citrate	20J26-B01-202653	1
Fagron	Sildenafil citrate	21B17-B09-203496	3
Fagron	Sildenafil citrate	21G10-B25	1
Fagron	Sildenafil citrate	21G10-B25-219206	2
Fagron	Sildenafil citrate	2OJ26-B01-201823	1
Fagron	Sildenafil citrate	B01-2018202	2
Fagron	Sildenafil citrate	BO9-2034906	1
Fargon	Sildenafil citrate	19B07-B02-194727	2
Gehe	Sildenafil citrate	13F24-N03	1
Gehe	Sildenafil citrate	16049805	1
GEHE	Sildenafil citrate	17344003	1
Gehe	Sildenafil citrate	17344008	1
Gehe	Sildenafil citrate	19086606	2
Gutenberg-Apotheke	Sildenafil citrate	1311010-01	1
Jenne	Sildenafil citrate	22000907015	1
Noweda/ Caesar & Lor…	Sildenafil citrate	19086607	1
Noweda	Sildenafil citrate	18B13-B06-347389	1
Noweda	Sildenafil citrate	18B13-B06-348002	1
Noweda	Sildenafil citrate	19086603	1
Noweda	Sildenafil citrate	19086607	1
Noweda	Sildenafil citrate	19B07-B02-194728	1
Noweda	Sildenafil citrate	19B07-BO2-191473	1
Noweda	Sildenafil citrate	SLC/0518011	1
ph euro	Sildenafil citrate	1908006-02	2
Phoenix	Sildenafil citrate	1311010-04	2
Phoenix	Sildenafil citrate	22000907015	1
Phönix	Sildenafil citrate	2003003-01	1
Phönix	Sildenafil citrate	22000907018	1
Phönix	Sildenafil citrate	473102016SC	1
Phönx/Polpharma	Sildenafil citrate	1311010-01	1
Polpharma/Phoenix	Sildenafil citrate	131101001	1
Sanacorp WE 21.04.17…	Sildenafil citrate	16049808	1
Sanacorp	Sildenafil citrate	14H11-B01-297519	2
Sanacorp	Sildenafil citrate	16049811	2
Sanacorp	Sildenafil citrate	19B07-b02-191473	1
Sanacorp	Sildenafil citrate	2003003-02	1
Sanacorp	Sildenafil citrate	2111002-01	1
Shangei tengben Biot…	Sildenafil citrate	20200110	1

- 235 324 spectra from 1515 *Apo-Ident* customers from a total of 49 053 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sildenafil citrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

relevant spectra of the various substances were compared with *Sildenafil citrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	540	0	201 544
Type C	0	742	1	235 324

The substance/substance group *Sildenafil citrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8889 %)
Type C	100.0000 % (> 99.9007 %)	99.8654 % (> 99.4616 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20852	20852	0.00	189.80
20927	20852	10.71	191.11
21621	24843	13.09	188.90
22446	22446	0.00	192.33
23178	23336	25.92	193.04
23336	23336	0.00	195.54
23345	23345	0.00	192.75
24843	24843	0.00	191.90

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Silver protein**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20178-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Silver protein; Argentum proteinicum

Special notes

When selecting the *Silver protein* substance/substance group, the following information is displayed to the user:

- Advice for the identification of silver protein: Silver protein acetyltannate is a similar substance, which is not included in the database. An additional analysis of identity may be required, e.g. identity test for Acetyl Ph. Eur. 2.3.1 - does not give a blue colour.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Silver protein	4	3	15

Second-stage model

For differentiation of the substance/substance group *Silver protein* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Silver protein* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	41.23	–
Polymyxin B sulfate	109.68	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Silver protein* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Silver protein*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Silver protein	190092	24559	40	20190221*
Caelo	Silver protein	22000752	26126	30	20220511*
Fagron	Silver protein	23D24-B08-229456	26820	40	20230512
Fagron	Silver protein	23J19-B03-235267	27037	40	20231108

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 150 spectra of 4 reference samples from the substance/substance group *Silver protein*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 812 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 6 reference samples from the substance/substance group *Silver protein*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Silver protein	21001315	25801	50
Caelo	Silver protein	24001987	27430	40
Fagron	Silver protein	24D17-B09-238717	27377	40
Caelo	Silver protein	22000752	26126SI†	20
Fagron	Silver protein	23D24-B08-229456	26820SI†	20
Fagron	Silver protein	23J19-B03-235267	27037SI†	20

- 201 894 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 40 spectra from 34 *Apo-Ident* customers from 15 batches from the substance/substance group *Silver protein*.
- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Silver protein	21001315005	1
	Silver protein	22000752007	2
	Silver protein	22001101018	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
	Silver protein	22F22-B01-220214	3
	Silver protein	23D24-B08-229465	1
	Silver protein	PTOR22-0172	1
2206030-01	Silver protein	2206030-01	1
Caelo	Silver protein	22000752001	3
Caelo	Silver protein	22000752003	6
Caelo	Silver protein	22000752004	1
Caelo	Silver protein	22000752005	1
Caelo	Silver protein	22000752006	1
Caelo	Silver protein	22000752007	2
Caesar & Loretz GmbH	Silver protein	22000752001	3
Caesar & Loretz GmbH	Silver protein	22000752003	1
Caesar & Loretz GmbH	Silver protein	22000752007	2
Euro OTC	Silver protein	2206030-01	1
Fagron	Silver protein	22D14B06216102	1
Fagron	Silver protein	22D14-B06-216102	1
Fagron	Silver protein	22F22-B01-220214	3
Fagron	Silver protein	PTOR22-0172	1
Gehe	Silver protein	22000752005	1
Noweda	Silver protein	22F22-B01-220214	1
Sanacorp	Silver protein	23D24-B08-233762	1

- 236 027 spectra from 1515 *Apo-Ident* customers from a total of 49 244 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Silver protein* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Silver protein* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	150	0	152 812
Type B	0	190	0	201 894
Type C	0	40	0	236 027

The substance/substance group *Silver protein* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 85.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24559	24559	0.00	50.75
26126	26126	0.00	30.91
26820	24559	17.73	43.68
27037	24559	15.53	53.47

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sodium acetate trihydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20984-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium acetate trihydrate; Natrii acetas trihydricum

Special notes

When selecting the *Sodium acetate trihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sodium acetate trihydrate	6	10	34

Second-stage model

For differentiation of the substance/substance group *Sodium acetate trihydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sodium acetate trihydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	56.86	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sodium acetate trihydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sodium acetate trihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium acetate trihydrate	12316506	20984	40	1402111
Caelo	Sodium acetate trihydrate	13411404	21441	60	20140113
Caelo	Sodium acetate trihydrate	172003	23812	40	20171107*
Euro OTC	Sodium acetate trihydrate	1507020	21861	60	20150723*
Euro OTC	Sodium acetate trihydrate	1706008	23547	40	20170710*
Euro OTC	Sodium acetate trihydrate	2002041	25131	40	20200331*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 280 spectra of 6 reference samples from the substance/substance group *Sodium acetate trihydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 682 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 490 spectra of 13 reference samples from the substance/substance group *Sodium acetate trihydrate*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium acetate trihydrate	163007	22760	40
Caelo	Sodium acetate trihydrate	183152	24370	40
Caelo	Sodium acetate trihydrate	21003448002	25983	40
Caelo	Sodium acetate trihydrate	22000375	26009	40
Caelo	Sodium acetate trihydrate	22003140	26478	30
Caelo	Sodium acetate trihydrate	24000576	27124	40
Euro OTC	Sodium acetate trihydrate	1608032	22802	40
Euro OTC	Sodium acetate trihydrate	1901026	24595	40
Euro OTC	Sodium acetate trihydrate	1906023	24811	40
Euro OTC	Sodium acetate trihydrate	2007023	25312	40
Caelo	Sodium acetate trihydrate	21003448002	25983SI	40
Caelo	Sodium acetate trihydrate	22000375	26009SI	40
Caelo	Sodium acetate trihydrate	22003140	26478SI	20

- 201 594 spectra from a total of 4036 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 91 spectra from 61 *Apo-Ident* customers from 36 batches from the substance/substance group *Sodium acetate trihydrate*.

- Among them are spectra of independent samples from 34 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sodium acetate trihydrate	21003723003	1
	Sodium acetate trihydrate	22000375003	1
	Sodium acetate trihydrate	22000375008	1
Anzag 02.11.20 6,55EUR	Sodium acetate trihydrate	220110NT	1
Caelo	Sodium acetate trihydrate	10353017	1
Caelo	Sodium acetate trihydrate	12027202	1
Caelo	Sodium acetate trihydrate	12027217	1
Caelo	Sodium acetate trihydrate	12027228	1
Caelo	Sodium acetate trihydrate	12316501	1
Caelo	Sodium acetate trihydrate	13295601	1
Caelo	Sodium acetate trihydrate	13295606	1
Caelo	Sodium acetate trihydrate	13411404	1
Caelo	Sodium acetate trihydrate	13411418	2
Caelo	Sodium acetate trihydrate	15118701	5
Caelo	Sodium acetate trihydrate	151452009	1
Caelo	Sodium acetate trihydrate	15145204	5
Caelo	Sodium acetate trihydrate	15145205	1
Caelo	Sodium acetate trihydrate	15145209	5
Caelo	Sodium acetate trihydrate	15145218	3
Caelo	Sodium acetate trihydrate	16300705	1
Caelo	Sodium acetate trihydrate	16300706	5
Caelo	Sodium acetate trihydrate	16300711	9
Caelo	Sodium acetate trihydrate	16300712	1
Caelo	Sodium acetate trihydrate	18006801	7
Caelo	Sodium acetate trihydrate	18173602	3
Caelo	Sodium acetate trihydrate	18315203	3
Caelo	Sodium acetate trihydrate	18315208	2
Caelo	Sodium acetate trihydrate	192116002	1
Caelo	Sodium acetate trihydrate	21000786002	3
Caelo	Sodium acetate trihydrate	21000786006	2
Caelo	Sodium acetate trihydrate	21003448002	2
Caelo	Sodium acetate trihydrate	22000375003	1
Caesar & Lorenz GmbH	Sodium acetate trihydrate	16300706	1
Caesar & Loretz GmbH…	Sodium acetate trihydrate	21003448002	1
Caesar & Loretz GmbH	Sodium acetate trihydrate	192116003	1
Caesar & Loretz GmbH	Sodium acetate trihydrate	21000786002	2
Caesar & Loretz GmbH	Sodium acetate trihydrate	21003448002	1
Caesar & Loretz GmbH	Sodium acetate trihydrate	22000375008	1
Ebert & Jacobi	Sodium acetate trihydrate	15145209	1
Ebert KKH 13.10.16	Sodium acetate trihydrate	15145204	1
Ebert KKH 13.10.16	Sodium acetate trihydrate	15145209	1
Euro OTC	Sodium acetate trihydrate	1005020V-01	1
Euro OTC	Sodium acetate trihydrate	2002041-01	1
Euro OTC	Sodium acetate trihydrate	2007023-01	1
Noweda	Sodium acetate trihydrate	21003723003	2
Phönix Gotha	Sodium acetate trihydrate	12316506	1
Sanacorp	Sodium acetate trihydrate	13295601	1

- 235 976 spectra from 1515 *Apo-Ident* customers from a total of 49 222 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Sodium acetate trihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sodium acetate trihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	490	0	201 594
Type C	0	91	0	235 976

The substance/substance group *Sodium acetate trihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.7755 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 93.4066 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20984	20984	0.00	95.57
21441	25131	9.08	98.45
21861	21861	0.00	84.63
23547	23547	0.00	90.02
23812	23812	0.00	91.58
25131	25131	0.00	102.88

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sodium ascorbate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20520-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium ascorbate; Natrii ascorbas

Special notes

When selecting the *Sodium ascorbate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sodium ascorbate	8	53	34

Second-stage model

For differentiation of the substance/substance group *Sodium ascorbate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sodium ascorbate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Aluminium chloride hexahydrate	88.66	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sodium ascorbate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sodium ascorbate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium ascorbate	15429905	22899	40	20160118
Caelo	Sodium ascorbate	182620	24386	40	20181112*
Caelo	Sodium ascorbate	20001049	25554	40	20200731*
Euro OTC	Sodium ascorbate	1406018-01	21583	60	1411165
Euro OTC	Sodium ascorbate	1406018-01	21789	60	20140724
Euro OTC	Sodium ascorbate	1507030	21853	60	20150811*
Euro OTC	Sodium ascorbate	1506018	21865	60	20150706*
Euro OTC	Sodium ascorbate	1510017	21946	60	20151102*
Euro OTC	Sodium ascorbate	1601007	22304	60	20160120*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 480 spectra of 9 reference samples from the substance/substance group *Sodium ascorbate*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 482 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 2419 spectra of 63 reference samples from the substance/substance group *Sodium ascorbate*.

- Among them are spectra of independent samples from 53 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium ascorbate	162857	22761	40
Caelo	Sodium ascorbate	172235	23809	40
Caelo	Sodium ascorbate	180326	24029	40
Caelo	Sodium ascorbate	191393	24751	40
Caelo	Sodium ascorbate	192304	24896	40
Caelo	Sodium ascorbate	22002242	26365	30
Caelo	Sodium ascorbate	23002840	27103	40
Caelo	Sodium ascorbate	24000403	27245	40
Caelo	Sodium ascorbate	24002134	27448	40
Euro OTC	Sodium ascorbate	1604001	22524	40
Euro OTC	Sodium ascorbate	1607044	22690	40
Euro OTC	Sodium ascorbate	1611015	22864	40
Euro OTC	Sodium ascorbate	1701054	23134	40
Euro OTC	Sodium ascorbate	1703012	23152	40
Euro OTC	Sodium ascorbate	1705013	23430	40
Euro OTC	Sodium ascorbate	1705014	23432	40
Euro OTC	Sodium ascorbate	1803005	24069	40
Euro OTC	Sodium ascorbate	1807043	24149	40
Euro OTC	Sodium ascorbate	1811002	24337	40
Euro OTC	Sodium ascorbate	1902021	24460	40
Euro OTC	Sodium ascorbate	1906005	24786	40
Euro OTC	Sodium ascorbate	1906004	24807	40
Euro OTC	Sodium ascorbate	1908026	24930	40
Euro OTC	Sodium ascorbate	2003024	25164	40
Euro OTC	Sodium ascorbate	2007008	25320	40
Euro OTC	Sodium ascorbate	2007009	25321	40
Euro OTC	Sodium ascorbate	2007010	25322	40
Euro OTC	Sodium ascorbate	2007011	25340	40
Euro OTC	Sodium ascorbate	2104010	25670	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Sodium ascorbate	2105016	25710	50
Euro OTC	Sodium ascorbate	2201001	25963	40
Euro OTC	Sodium ascorbate	2201002	25965	40
Euro OTC	Sodium ascorbate	2205026	26187	40
Euro OTC	Sodium ascorbate	2205025	26193	40
Euro OTC	Sodium ascorbate	2208013	26274	40
Euro OTC	Sodium ascorbate	2208014	26278	39
Euro OTC	Sodium ascorbate	2211010	26420	40
Euro OTC	Sodium ascorbate	2211011	26441	40
Euro OTC	Sodium ascorbate	2308007	26933	40
Euro OTC	Sodium ascorbate	2308009	26935	40
Euro OTC	Sodium ascorbate	2308008	26936	40
Euro OTC	Sodium ascorbate	2402016	27197	40
Euro OTC	Sodium ascorbate	2402011	27199	40
Euro OTC	Sodium ascorbate	2402014	27201	40
Euro OTC	Sodium ascorbate	2402015	27202	40
Euro OTC	Sodium ascorbate	2402001	27270	40
Euro OTC	Sodium ascorbate	2402002	27271	40
Euro OTC	Sodium ascorbate	2402003	27272	40
Euro OTC	Sodium ascorbate	2402010	27273	40
Euro OTC	Sodium ascorbate	2402005	27356	40
Euro OTC	Sodium ascorbate	2402004	27357	40
Euro OTC	Sodium ascorbate	2402006	27358	40
Euro OTC	Sodium ascorbate	2402007	27359	40
Caelo	Sodium ascorbate	22002242	26365SI	20
Euro OTC	Sodium ascorbate	1906004	24935	40
Euro OTC	Sodium ascorbate	1902021	24943	40
Euro OTC	Sodium ascorbate	1906005	24976	40
Euro OTC	Sodium ascorbate	2201001	25963SI	40
Euro OTC	Sodium ascorbate	2201002	25965SI	40
Euro OTC	Sodium ascorbate	2205026	26187SI	20
Euro OTC	Sodium ascorbate	2205025	26193SI	20
Euro OTC	Sodium ascorbate	2208013	26274SI	20
Euro OTC	Sodium ascorbate	2208014	26278SI	20

- 199 665 spectra from a total of 3992 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 43 spectra from 16 *Apo-Ident* customers from 34 batches from the substance/substance group *Sodium ascorbate*.
- Among them are spectra of independent samples from 34 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Sodium ascorbate	14079404	1
Caelo	Sodium ascorbate	15180505	1
Caelo	Sodium ascorbate	15429917	1
Caelo	Sodium ascorbate	1604001-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sodium ascorbate	1628505	1
Caelo	Sodium ascorbate	16285710	1
Caelo	Sodium ascorbate	17223504	1
Caelo	Sodium ascorbate	17356201	1
Caelo	Sodium ascorbate	27091302	1
Caesar & Loretz GmbH/gehe	Sodium ascorbate	19139304	1
Caesar & Loretz GmbH	Sodium ascorbate	18262001	1
Caesar & Loretz GmbH	Sodium ascorbate	18262009	1
Caesar & Loretz GmbH	Sodium ascorbate	21001574004	2
Caesar & Loretz GmbH	Sodium ascorbate	21003620003	1
Euro OTC	Sodium ascorbate	11081401	1
Euro OTC	Sodium ascorbate	11121301	1
Euro OTC	Sodium ascorbate	12061407	1
Euro OTC	Sodium ascorbate	1210026-01	1
Euro OTC	Sodium ascorbate	13031402	1
Euro OTC	Sodium ascorbate	13051406	1
Euro OTC	Sodium ascorbate	16091301	1
Euro OTC	Sodium ascorbate	170105401	1
Euro OTC	Sodium ascorbate	1703012-01	1
Euro OTC	Sodium ascorbate	200708-01	1
Euro OTC	Sodium ascorbate	20091303	1
Euro OTC	Sodium ascorbate	2208013-01	2
Euro OTC	Sodium ascorbate	28081304	1
Euro OTC	Sodium ascorbate	4021401	1
Euro OTC	Sodium ascorbate	7011405	1
Euro OTC	Sodium ascorbate	L1308005-01	1
Fagron	Sodium ascorbate	12L27-N03	1
Fagron	Sodium ascorbate	13C15-N01	1
Gatt-Koller	Sodium ascorbate	1802317	3
Pharma Greven	Sodium ascorbate	HPN1904025	6

- 236 024 spectra from 1515 *Apo-Ident* customers from a total of 49 224 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sodium ascorbate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sodium ascorbate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	480	0	152 482
Type B	0	2419	0	199 665
Type C	0	43	0	236 024

The substance/substance group *Sodium ascorbate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.7520 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 86.0465 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21583	21583	0.00	158.39
21789	21865	4.16	181.17
21853	21853	0.00	175.26
21865	21865	0.00	177.93
21946	21946	0.00	171.91
22304	22304	0.00	185.95
22899	22304	4.37	187.01
24386	24386	0.00	185.12
25554	25554	0.00	186.34

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sodium benzoate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10006331-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium benzoate; Natrii benzoas

Special notes

When selecting the *Sodium benzoate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sodium benzoate	11	17	185

Second-stage model

For differentiation of the substance/substance group *Sodium benzoate* the following second-stage model is used:

- Submodel 18

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sodium benzoate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Diphenylcyclopropenone	53.35	16.56

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sodium benzoate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sodium benzoate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium benzoate	11267016	20752	40	20110923
Caelo	Sodium benzoate	13178619	21607	60	20130624
Euro OTC	Sodium benzoate	1409040-01	21713	60	20141021
Euro OTC	Sodium benzoate	1506019	21825	60	20150623*
Euro OTC	Sodium benzoate	1510044	22236	60	20151109*
Euro OTC	Sodium benzoate	1602020	22363	60	20160225*
Euro OTC	Sodium benzoate	1610037	22867	40	20161202*
Euro OTC	Sodium benzoate	1701045	22997	40	20170207*
Euro OTC	Sodium benzoate	1711019	23900	40	20171205*
Euro OTC	Sodium benzoate	2001018	25081	40	20200205*
Euro OTC	Sodium benzoate	2009005	25379	40	20201001*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 540 spectra of 11 reference samples from the substance/substance group *Sodium benzoate*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 422 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 790 spectra of 21 reference samples from the substance/substance group *Sodium benzoate*.

- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium benzoate	161371	22474	60
Caelo	Sodium benzoate	170558	23283	40
Caelo	Sodium benzoate	173530	23784	40
Caelo	Sodium benzoate	190541	24544	40
Caelo	Sodium benzoate	21001722	25805	50
Caelo	Sodium benzoate	22001421	26253	40
Caelo	Sodium benzoate	24001874	27336	40
Euro OTC	Sodium benzoate	1607005	22670	40
Euro OTC	Sodium benzoate	1707024	23613	40
Euro OTC	Sodium benzoate	1803034	24068	40
Euro OTC	Sodium benzoate	1809005	24301	40
Euro OTC	Sodium benzoate	1901043	24481	40
Euro OTC	Sodium benzoate	2109016	25893	50
Euro OTC	Sodium benzoate	2207025	26269	40
Euro OTC	Sodium benzoate	2302017	26583	40
Euro OTC	Sodium benzoate	2308011	26908	40
Fagron	Sodium benzoate	15B16-B07-308570	22895	40
Caelo	Sodium benzoate	22001421	26253SI	20
Euro OTC	Sodium benzoate	2109016	25893SI	10
Euro OTC	Sodium benzoate	2207025	26269SI	20
Euro OTC	Sodium benzoate	2302017	26583SI	20

- 201 294 spectra from a total of 4028 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 936 spectra from 573 *Apo-Ident* customers from 194 batches from the substance/substance group *Sodium benzoate*.
- Among them are spectra of independent samples from 185 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sodium benzoate	2009005	1
	Sodium benzoate	2109016-01	1
	Sodium benzoate	22001421002	3
	Sodium benzoate	22001421009	2
	Sodium benzoate	22001421011	1
	Sodium benzoate	22001421014	4
	Sodium benzoate	22001421021	2
	Sodium benzoate	2200142104	1
	Sodium benzoate	2207025-01	1
	Sodium benzoate	2308011-01	4
	Sodium benzoate	2308011-02	2
AHD	Sodium benzoate	1711019-01	3
AHD	Sodium benzoate	17137606	1
AHD	Sodium benzoate	192296011	1
AHD	Sodium benzoate	2308011-02	1
Alliance Healthcare	Sodium benzoate	1304024-01	1
Alliance Healthcare	Sodium benzoate	2207025-01	1
Alliance/EurRho	Sodium benzoate	2009005-01	1
Alliance	Sodium benzoate	2009005-01	1
Anzag	Sodium benzoate	20003762002	1
Anzag	Sodium benzoate	20003762010	3
Anzag	Sodium benzoate	21001722009	2
Bombastus	Sodium benzoate	1404011-01	1
Bombastus	Sodium benzoate	17055805	1
Bombastus	Sodium benzoate	17353011	1
Caela/Phoenix	Sodium benzoate	19054114	2
Caelo	Sodium benzoate		1
Caelo	Sodium benzoate	10003762015	1
Caelo	Sodium benzoate	10544104	1
Caelo	Sodium benzoate	11267016	1
Caelo	Sodium benzoate	11346109	3
Caelo	Sodium benzoate	1209018-0	1
Caelo	Sodium benzoate	12158401	1
Caelo	Sodium benzoate	12158418	1
Caelo	Sodium benzoate	12158419	4
Caelo	Sodium benzoate	12158424	1
Caelo	Sodium benzoate	12158439	4
Caelo	Sodium benzoate	12J23-N05	1
Caelo	Sodium benzoate	13178603	2
Caelo	Sodium benzoate	13178605	3
Caelo	Sodium benzoate	13178613	1
Caelo	Sodium benzoate	13178619	2
Caelo	Sodium benzoate	13178627	1
Caelo	Sodium benzoate	13178635	5
Caelo	Sodium benzoate	13178647	2
Caelo	Sodium benzoate	13H01-N02	1
Caelo	Sodium benzoate	14166714	1
Caelo	Sodium benzoate	14328702	1
Caelo	Sodium benzoate	1503022-01	1
Caelo	Sodium benzoate	15044102	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sodium benzoate	15044104	9
Caelo	Sodium benzoate	1506019-01	1
Caelo	Sodium benzoate	151208NB	1
Caelo	Sodium benzoate	15135001	7
Caelo	Sodium benzoate	15363401	12
Caelo	Sodium benzoate	15363409	3
Caelo	Sodium benzoate	15363413	2
Caelo	Sodium benzoate	15363414	1
Caelo	Sodium benzoate	15363424	11
Caelo	Sodium benzoate	1610037-01	1
Caelo	Sodium benzoate	161371	1
Caelo	Sodium benzoate	16137103	12
Caelo	Sodium benzoate	16137104	2
Caelo	Sodium benzoate	16137112	6
Caelo	Sodium benzoate	16137118	9
Caelo	Sodium benzoate	17055801	5
Caelo	Sodium benzoate	17055805	6
Caelo	Sodium benzoate	17055806	1
Caelo	Sodium benzoate	17061306	1
Caelo	Sodium benzoate	17137603	1
Caelo	Sodium benzoate	17137604	3
Caelo	Sodium benzoate	17137606	18
Caelo	Sodium benzoate	17137607	1
Caelo	Sodium benzoate	17137609	1
Caelo	Sodium benzoate	1735011	2
Caelo	Sodium benzoate	17353001	22
Caelo	Sodium benzoate	17353002	1
Caelo	Sodium benzoate	17353006	2
Caelo	Sodium benzoate	17353011	12
Caelo	Sodium benzoate	18055805	1
Caelo	Sodium benzoate	18161201	17
Caelo	Sodium benzoate	18161202	1
Caelo	Sodium benzoate	18161209	1
Caelo	Sodium benzoate	18161211	22
Caelo	Sodium benzoate	18161214	1
Caelo	Sodium benzoate	1827	1
Caelo	Sodium benzoate	1901043-02	1
Caelo	Sodium benzoate	19054104	10
Caelo	Sodium benzoate	19054105	4
Caelo	Sodium benzoate	19054106	1
Caelo	Sodium benzoate	19054114	20
Caelo	Sodium benzoate	19091801	1
Caelo	Sodium benzoate	191031709	1
Caelo	Sodium benzoate	192296003	27
Caelo	Sodium benzoate	192296004	1
Caelo	Sodium benzoate	192296011	10
Caelo	Sodium benzoate	192296015	12
Caelo	Sodium benzoate	192296016	7
Caelo	Sodium benzoate	20001291001	2
Caelo	Sodium benzoate	20001291005	7
Caelo	Sodium benzoate	2000376007	1
Caelo	Sodium benzoate	2000376009	1
Caelo	Sodium benzoate	20003762003	12
Caelo	Sodium benzoate	20003762007	10
Caelo	Sodium benzoate	20003762009	30
Caelo	Sodium benzoate	20003762010	1
Caelo	Sodium benzoate	20003762013	3
Caelo	Sodium benzoate	20003762015	4
Caelo	Sodium benzoate	20003792010	1
Caelo	Sodium benzoate	2001291001	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sodium benzoate	210014722004	1
Caelo	Sodium benzoate	21001722003	9
Caelo	Sodium benzoate	21001722006	11
Caelo	Sodium benzoate	21001722008	20
Caelo	Sodium benzoate	21001722020	4
Caelo	Sodium benzoate	2100172203	2
Caelo	Sodium benzoate	2100172206	1
Caelo	Sodium benzoate	2109016-01	1
Caelo	Sodium benzoate	2200142002	1
Caelo	Sodium benzoate	22001421002	13
Caelo	Sodium benzoate	22001421009	2
Caelo	Sodium benzoate	22001421014	3
Caelo	Sodium benzoate	2215Q-01891	1
Caelo	Sodium benzoate	24021501	1
Caelo	Sodium benzoate	3037647	1
Caelo	Sodium benzoate	3918M-01891	1
Caelo	Sodium benzoate	4315A-01891	1
Caelo	Sodium benzoate	5117A-01891	1
Caelo	Sodium benzoate	5211I-01891	1
Caelo	Sodium benzoate	91443209	2
Caelo	Sodium benzoate	NB20180313	1
Caesar & Loretz GmbH...	Sodium benzoate	19054114	1
Caesar & Loretz GmbH...	Sodium benzoate	21001722008	1
Caesar & Loretz GmbH...	Sodium benzoate	20003762013	1
Caesar & Loretz GmbH...	Sodium benzoate	21001722003	2
Caesar & Loretz GmbH...	Sodium benzoate	19054114	1
Caesar & Loretz GmbH...	Sodium benzoate	21001722003	1
Caesar & Loretz GmbH...	Sodium benzoate	192296011	1
Caesar & Loretz GmbH/AHD	Sodium benzoate	20003762013	1
Caesar & Loretz GmbH...	Sodium benzoate	192296003	1
Caesar & Loretz GmbH/E	Sodium benzoate	20003762007	1
Caesar & Loretz GmbH...	Sodium benzoate	19054104	1
Caesar & Loretz GmbH...	Sodium benzoate	20003762009	1
Caesar & Loretz GmbH/GEHE	Sodium benzoate	192296003	1
Caesar & Loretz GmbH/Gehe	Sodium benzoate	192296015	2
Caesar & Loretz GmbH/Gehe	Sodium benzoate	20003762002	2
Caesar & Loretz GmbH/Gehe	Sodium benzoate	20003762010	1
Caesar & Loretz GmbH...	Sodium benzoate	19054114	1
Caesar & Loretz GmbH...	Sodium benzoate	20003762009	1
Caesar & Loretz GmbH...	Sodium benzoate	21001722003	1
Caesar & Loretz GmbH...	Sodium benzoate	21001722008	1
Caesar & Loretz GmbH...	Sodium benzoate	20003762009	1
Caesar & Loretz GmbH...	Sodium benzoate	20001291005	1
Caesar & Loretz GmbH...	Sodium benzoate	20003762013	1
Caesar & Loretz GmbH	Sodium benzoate	18161201	1
Caesar & Loretz GmbH	Sodium benzoate	18161211	1
Caesar & Loretz GmbH	Sodium benzoate	19054104	2
Caesar & Loretz GmbH	Sodium benzoate	19054114	4
Caesar & Loretz GmbH	Sodium benzoate	192296003	3
Caesar & Loretz GmbH	Sodium benzoate	192296011	5
Caesar & Loretz GmbH	Sodium benzoate	192296015	3
Caesar & Loretz GmbH	Sodium benzoate	20001291001	3
Caesar & Loretz GmbH	Sodium benzoate	20001291005	3
Caesar & Loretz GmbH	Sodium benzoate	20003762003	7
Caesar & Loretz GmbH	Sodium benzoate	20003762007	6
Caesar & Loretz GmbH	Sodium benzoate	20003762009	8
Caesar & Loretz GmbH	Sodium benzoate	20003762013	3
Caesar & Loretz GmbH	Sodium benzoate	21001722003	5
Caesar & Loretz GmbH	Sodium benzoate	21001722004	2
Caesar & Loretz GmbH	Sodium benzoate	21001722006	9

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Sodium benzoate	21001722008	7
Caesar & Loretz GmbH	Sodium benzoate	21001722009	2
Caesar & Loretz GmbH	Sodium benzoate	21001722020	3
Caesar & Loretz GmbH	Sodium benzoate	22001421001	3
Caesar & Loretz GmbH	Sodium benzoate	22001421002	3
Caesar & Loretz Hilden	Sodium benzoate	18161201	1
Caesar&Lorenz	Sodium benzoate	20003762015	1
Calo/Krieger	Sodium benzoate	19054104	1
calo	Sodium benzoate	17055805	1
Chiesi/Krieger	Sodium benzoate	17353011	1
EuRho / Noweda	Sodium benzoate	2009005-01	1
EuRho / Phoenix	Sodium benzoate	2001018-01	1
EuRho Anzag	Sodium benzoate	1304024-01	1
EuRho/Sanacorp	Sodium benzoate	190104302	1
EuRho	Sodium benzoate	1112006-01	1
EuRho	Sodium benzoate	2009005-01	1
Euro OCT / Noweda	Sodium benzoate	1510044-01	1
Euro OTC	Sodium benzoate	1007019-01	1
Euro OTC	Sodium benzoate	1112006-01	1
Euro OTC	Sodium benzoate	1209018-01	4
Euro OTC	Sodium benzoate	1209018-18	1
Euro OTC	Sodium benzoate	130402401	2
Euro OTC	Sodium benzoate	1304024-01	6
Euro OTC	Sodium benzoate	1307013-01	2
Euro OTC	Sodium benzoate	1309027-01	2
Euro OTC	Sodium benzoate	14040-01	1
Euro OTC	Sodium benzoate	1404011-01	4
Euro OTC	Sodium benzoate	1409040-01	2
Euro OTC	Sodium benzoate	15060119-01	1
Euro OTC	Sodium benzoate	1506019-01	7
Euro OTC	Sodium benzoate	151004401	4
Euro OTC	Sodium benzoate	1510044-01	15
Euro OTC	Sodium benzoate	1510044-0104932321	1
Euro OTC	Sodium benzoate	15363424	1
Euro OTC	Sodium benzoate	1602020-01	2
Euro OTC	Sodium benzoate	1607005-01	5
Euro OTC	Sodium benzoate	161003701	1
Euro OTC	Sodium benzoate	1610037-01	3
Euro OTC	Sodium benzoate	16137112	1
Euro OTC	Sodium benzoate	1701045	1
Euro OTC	Sodium benzoate	1701045-01	5
Euro OTC	Sodium benzoate	170702401	1
Euro OTC	Sodium benzoate	1707024-01	3
Euro OTC	Sodium benzoate	171101901	1
Euro OTC	Sodium benzoate	1711019-01	3
Euro OTC	Sodium benzoate	1803034-01	3
Euro OTC	Sodium benzoate	1809005	1
Euro OTC	Sodium benzoate	180900501	2
Euro OTC	Sodium benzoate	1809005-01	22
Euro OTC	Sodium benzoate	1841	1
Euro OTC	Sodium benzoate	1901043	1
Euro OTC	Sodium benzoate	190104301	1
Euro OTC	Sodium benzoate	1901043-01	9
Euro OTC	Sodium benzoate	1901043-02	11
Euro OTC	Sodium benzoate	2001018	1
Euro OTC	Sodium benzoate	200101801	1
Euro OTC	Sodium benzoate	2001018-01	13
Euro OTC	Sodium benzoate	20010-18-01	1
Euro OTC	Sodium benzoate	200900501	1
Euro OTC	Sodium benzoate	2009005-01	17

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Sodium benzoate	210901601	1
Euro OTC	Sodium benzoate	2109016-01	9
Euro OTC	Sodium benzoate	2109016-02	1
Euro OTC	Sodium benzoate	2132	1
Euro OTC	Sodium benzoate	2207025-01	1
Euro OTC	Sodium benzoate	2302017-01	1
Euro OTC	Sodium benzoate	2604040V-05	1
Euro Rho	Sodium benzoate	1803034-01	1
Euro/ Phönix	Sodium benzoate	1404011-01	1
EuroTOC / Noweda	Sodium benzoate	130902701	1
Fagron	Sodium benzoate	12C05-N04	1
Fagron	Sodium benzoate	12D02-N06	1
Fagron	Sodium benzoate	12G04-N04	1
Fagron	Sodium benzoate	12H08-N06	1
Fagron	Sodium benzoate	12J23-N05	3
Fagron	Sodium benzoate	13/27b03288805	1
Fagron	Sodium benzoate	13/27B03288805	1
Fagron	Sodium benzoate	13/27-B03-288805	1
Fagron	Sodium benzoate	13/27-B03-288806	2
Fagron	Sodium benzoate	13C14-N01	4
Fagron	Sodium benzoate	13C14-NO1	1
Fagron	Sodium benzoate	13H01-N02	1
Fagron	Sodium benzoate	13I27-B03288805	1
Fagron	Sodium benzoate	13I27-B03-288806	3
Fagron	Sodium benzoate	13l27-B03-288806	1
Fagron	Sodium benzoate	1412	1
Fagron	Sodium benzoate	14E12-B07	1
Fagron	Sodium benzoate	14E12B07296717	1
Fagron	Sodium benzoate	14E12-B07-306570	1
Fagron	Sodium benzoate	14E12Bo7296717	1
Fagron	Sodium benzoate	14E12BO7296717	1
Fagron	Sodium benzoate	1510044-01	2
Fagron	Sodium benzoate	15363403	1
Fagron	Sodium benzoate	15B16-B07	1
Fagron	Sodium benzoate	15B16-B07-306571	2
Fagron	Sodium benzoate	15B16-B07-308570	1
Fagron	Sodium benzoate	1602020-01	1
Fagron	Sodium benzoate	16B23-B06-322528	1
Fagron	Sodium benzoate	24011401	1
Fagron	Sodium benzoate	test	1
Fiebig 27.06.13 EK3,34	Sodium benzoate	1304024-01	1
Gehe	Sodium benzoate	1404011-01	1
Gehe	Sodium benzoate	15044102	1
Gehe	Sodium benzoate	1610037-01	1
Gehe	Sodium benzoate	1707024-01	2
GEHE	Sodium benzoate	17137606	1
Gehe	Sodium benzoate	17317606	1
GEHE	Sodium benzoate	17353006	2
Gehe	Sodium benzoate	18161211	7
Gehe	Sodium benzoate	21001722006	1
Gehe	Sodium benzoate	2109016-01	1
Gehe	Sodium benzoate	22001421009	1
Hedinger/Phönix	Sodium benzoate	15363413	1
Hedinger	Sodium benzoate	13I27-B03	1
Jenne	Sodium benzoate	20003762007	1
Kehr	Sodium benzoate	1701045-01	1
Nachtestung	Sodium benzoate	300/18	1
Nokun	Sodium benzoate	17137606	2
Noweda	Sodium benzoate	1209018-01	1
Noweda	Sodium benzoate	16137103	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Sodium benzoate	16137112	1
Noweda	Sodium benzoate	1711019-01	1
Noweda	Sodium benzoate	18161201	1
Noweda	Sodium benzoate	189005-01	1
Noweda	Sodium benzoate	1901043-02	2
Noweda	Sodium benzoate	192296016	1
Pala	Sodium benzoate	192296003	1
Phoenix goettin	Sodium benzoate	13I27-B03-288806	1
Phoenix	Sodium benzoate	1610037-01	1
Phoenix	Sodium benzoate	2003762009	1
Phoenix	Sodium benzoate	2201421009	1
Phönix Gotha	Sodium benzoate	18161211	2
Phönix Gotha	Sodium benzoate	19054114	1
Phönix	Sodium benzoate	1510044/01	1
Phönix	Sodium benzoate	17137606	1
Phönix	Sodium benzoate	18161201	1
Phönix	Sodium benzoate	192296004	2
Phönix	Sodium benzoate	192296015	1
Phönix	Sodium benzoate	20001291001	3
sana	Sodium benzoate	13178635	1
Sanacorp	Sodium benzoate	192296015	1
Sanacorp	Sodium benzoate	20001291005	1
Sanacorp	Sodium benzoate	22001421009	1
Unisan	Sodium benzoate	1404011-01	1

- 235 131 spectra from 1515 *Apo-Ident* customers from a total of 49 066 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sodium benzoate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sodium benzoate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	540	0	152 422
Type B	0	790	0	201 294
Type C	0	935	1	235 131

The substance/substance group *Sodium benzoate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8889 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2405 %)
Type C	100.0000 % (> 99.9007 %)	99.8932 % (> 99.5726 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20752	22236	20.96	163.63
21607	22363	13.56	160.28
21713	22236	15.14	164.84
21825	21825	0.00	152.10
22236	22236	0.00	166.43
22363	22363	0.00	155.50
22867	22867	0.00	156.41
22997	22997	0.00	156.42
23900	23900	0.00	151.29
25081	25081	0.00	153.98
25379	25379	0.00	213.47

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sodium chondroitin sulfate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	24283-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium chondroitin sulfate; Sodium chondroitin sulphate

Special notes

When selecting the *Sodium chondroitin sulfate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sodium chondroitin sulfate	2	1	0

Second-stage model

For differentiation of the substance/substance group *Sodium chondroitin sulfate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sodium chondroitin sulfate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	59.57	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sodium chondroitin sulfate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sodium chondroitin sulfate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Yino Pharma	Sodium chondroitin sulfate	YN010511806006	24284	40	20180912*
Yino Pharma	Sodium chondroitin sulfate	YN010511805005	24285	40	20180912*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 80 spectra of 2 reference samples from the substance/substance group *Sodium chondroitin sulfate*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 882 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Sodium chondroitin sulfate*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Yino Pharma	Sodium chondroitin sulfate	YN010511806007	24283	40

- 202 044 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Sodium chondroitin sulfate*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sodium chondroitin sulfate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sodium chondroitin sulfate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	80	0	152 882
Type B	0	40	0	202 044
Type C	0	0	0	236 067

The substance/substance group *Sodium chondroitin sulfate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 92.5000 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24284	24284	0.00	75.84
24285	24285	0.00	70.59

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sodium citrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20662-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium citrate; Natrii citras

Special notes

When selecting the *Sodium citrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sodium citrate	11	19	410

Second-stage model

For differentiation of the substance/substance group *Sodium citrate* the following second-stage model is used:

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sodium citrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	50.17	–
⋮	⋮	⋮
Capsaicin	>50	137.69
Heparin sodium	>50	173.89
Sucrose	>50	221.71
Quinine hydrochloride dihydrate	>50	256.66
Pyridoxal-5-phosphate	>50	304.46
Levocarnitine	>50	333.14
Oxybutynin hydrochloride	>50	348.28
Amifampridine	>50	429.64
Alfatradiol	>50	435.17
Prednicarbate	>50	504.61
Ciprofloxacin hydrochloride	>50	594.85
Triclosan	>50	613.22
Methoxsalen	>50	651.06
Tetracaine	>50	773.85
Cyproterone acetate	>50	1008.42
Norethisterone acetate	>50	1165.10
Amitriptyline hydrochloride	>50	2069.28
Valine	>50	2706.92

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sodium citrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sodium citrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium citrate	12045026	20918	40	20120307
Caelo	Sodium citrate	13089335	21670	60	AR-15-FG-000405-01

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium citrate	14112517	21718	60	20140416
Euro OTC	Sodium citrate	1506041	21839	60	0000010492
Euro OTC	Sodium citrate	1511017	21997	60	20151130*
Euro OTC	Sodium citrate	1610016	22859	40	20161102*
Euro OTC	Sodium citrate	1701029	22996	40	20170126*
Euro OTC	Sodium citrate	2007022	25324	40	20200820*
Fagron	Sodium citrate	12E04-N05	20662	40	20120516
Fagron	Sodium citrate	14A13-B02-294541	21778	60	20140424
Fagron	Sodium citrate	16F10-B01-326088	22843	40	20160711

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 540 spectra of 11 reference samples from the substance/substance group *Sodium citrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.
- 152 422 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 810 spectra of 22 reference samples from the substance/substance group *Sodium citrate*.
- Among them are spectra of independent samples from 19 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium citrate	162179	22618	40
Caelo	Sodium citrate	173236	23789	40
Caelo	Sodium citrate	182083	24218	40
Caelo	Sodium citrate	190890	24533	40
Caelo	Sodium citrate	20002150	25229	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium citrate	22002778	26501	40
Euro OTC	Sodium citrate	1604030	22510	40
Euro OTC	Sodium citrate	1607040	22687	40
Euro OTC	Sodium citrate	1710006	23614	40
Euro OTC	Sodium citrate	1807035	24151	40
Euro OTC	Sodium citrate	1901035	24487	40
Euro OTC	Sodium citrate	1909020	24862	40
Euro OTC	Sodium citrate	2002040	25127	40
Euro OTC	Sodium citrate	2101007	25550	40
Euro OTC	Sodium citrate	2206011	26221	40
Euro OTC	Sodium citrate	2212001	26419	30
Euro OTC	Sodium citrate	2307019	26862	40
Fagron	Sodium citrate	22A15-B18-219203	26154	40
Fagron	Sodium citrate	22K17-B15-223095	26983	40
Caelo	Sodium citrate	22002778	26501SI	20
Euro OTC	Sodium citrate	2206011	26221SI	20
Fagron	Sodium citrate	22A15-B18-219203	26154SI	20

- 201 274 spectra from a total of 4026 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2248 spectra from 998 *Apo-Ident* customers from 423 batches from the substance/substance group *Sodium citrate*.

- Among them are spectra of independent samples from 409 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sodium citrate		1
	Sodium citrate	1710006-01	1
	Sodium citrate	18208302	1
	Sodium citrate	190890007	1
	Sodium citrate	21002580012	1
	Sodium citrate	21002580018	1
	Sodium citrate	21002580019	1
	Sodium citrate	2101007-01	1
	Sodium citrate	22002778001	1
	Sodium citrate	22002778003	3
	Sodium citrate	22002778007	17
	Sodium citrate	22002778008	1
	Sodium citrate	2212001-001	1
	Sodium citrate	2212001-01	13
	Sodium citrate	2212001-02	1
	Sodium citrate	2212001-03	1
	Sodium citrate	23000473002	11
	Sodium citrate	23003487003	5
	Sodium citrate	3118872	2
AHD	Sodium citrate	1710006-01	2
AHD	Sodium citrate	17323602	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
AHD	Sodium citrate	1901035-01	1
AHD	Sodium citrate	22002778003	1
Alli	Sodium citrate	22002778007	1
Alliance Healthcare	Sodium citrate	1211030-01	1
Alliance	Sodium citrate	22002778003	1
Anzag	Sodium citrate	1512705	1
Anzag	Sodium citrate	20A20-F03-369331	1
Anzag	Sodium citrate	21002580012	1
Anzag	Sodium citrate	2212001-01	1
ApoIdent/ Phoenix	Sodium citrate	1710006-01	1
apo-ident	Sodium citrate	1701029-01	1
Apo-ident	Sodium citrate	3065202	1
Audor Pharma	Sodium citrate	171000601	1
Aug. Hedinger	Sodium citrate	8765456	1
Bombastus	Sodium citrate	73155098	1
Caelo	Sodium citrate		15
Caelo	Sodium citrate	1042	1
Caelo	Sodium citrate	1107011-01	1
Caelo	Sodium citrate	11081514	1
Caelo	Sodium citrate	11121303	1
Caelo	Sodium citrate	11219012	6
Caelo	Sodium citrate	1123588946	1
Caelo	Sodium citrate	11304311	3
Caelo	Sodium citrate	1151351	2
Caelo	Sodium citrate	1161207	2
Caelo	Sodium citrate	1200002828764	1
Caelo	Sodium citrate	12045001	1
Caelo	Sodium citrate	12045002	1
Caelo	Sodium citrate	12045004	4
Caelo	Sodium citrate	12045006	1
Caelo	Sodium citrate	12045008	4
Caelo	Sodium citrate	12045011	6
Caelo	Sodium citrate	12045012	1
Caelo	Sodium citrate	12045016	5
Caelo	Sodium citrate	12045016-3451311172	1
Caelo	Sodium citrate	12045019	4
Caelo	Sodium citrate	12045024	5
Caelo	Sodium citrate	12045026	7
Caelo	Sodium citrate	1223test	1
Caelo	Sodium citrate	1234	3
Caelo	Sodium citrate	123456	2
Caelo	Sodium citrate	1234567	1
Caelo	Sodium citrate	123456789	1
Caelo	Sodium citrate	1234test	1
Caelo	Sodium citrate	1234Test	3
Caelo	Sodium citrate	12358Test	1
Caelo	Sodium citrate	123658	1
Caelo	Sodium citrate	123e2	1
Caelo	Sodium citrate	123test	6
Caelo	Sodium citrate	123Test	16
Caelo	Sodium citrate	123tst	1
Caelo	Sodium citrate	1256825	1
Caelo	Sodium citrate	125874566	1
Caelo	Sodium citrate	128896	1
Caelo	Sodium citrate	12897	1
Caelo	Sodium citrate	13/24-B13-287921	1
Caelo	Sodium citrate	1308908	1
Caelo	Sodium citrate	13089304	2
Caelo	Sodium citrate	13089305	1
Caelo	Sodium citrate	13089308	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sodium citrate	13089314	1
Caelo	Sodium citrate	13089317	7
Caelo	Sodium citrate	13089319	4
Caelo	Sodium citrate	13089325	3
Caelo	Sodium citrate	13089329	1
Caelo	Sodium citrate	13089331	5
Caelo	Sodium citrate	13089335	8
Caelo	Sodium citrate	131103501	1
Caelo	Sodium citrate	1319A-01900	1
Caelo	Sodium citrate	1404033-01	3
Caelo	Sodium citrate	140510/1	1
Caelo	Sodium citrate	140731NC	1
Caelo	Sodium citrate	14112502	26
Caelo	Sodium citrate	14112517	12
Caelo	Sodium citrate	14112518	1
Caelo	Sodium citrate	14112520	1
Caelo	Sodium citrate	1411502	1
Caelo	Sodium citrate	1412014-01	1
Caelo	Sodium citrate	14360407	1
Caelo	Sodium citrate	14369402	2
Caelo	Sodium citrate	14369406	9
Caelo	Sodium citrate	14369407	51
Caelo	Sodium citrate	14369411	3
Caelo	Sodium citrate	14369413	22
Caelo	Sodium citrate	14369414	1
Caelo	Sodium citrate	14369415	1
Caelo	Sodium citrate	14369416	1
Caelo	Sodium citrate	14369423	21
Caelo	Sodium citrate	14369424	4
Caelo	Sodium citrate	1469413	1
Caelo	Sodium citrate	14838	1
Caelo	Sodium citrate	14A13-B02_300395	1
Caelo	Sodium citrate	1506041-01	1
Caelo	Sodium citrate	151101701	1
Caelo	Sodium citrate	1511017-01	3
Caelo	Sodium citrate	15212705	5
Caelo	Sodium citrate	154662	1
Caelo	Sodium citrate	15C27-B01-309893	1
Caelo	Sodium citrate	160704001	1
Caelo	Sodium citrate	1607040-01	4
Caelo	Sodium citrate	160955707	1
Caelo	Sodium citrate	16095702	4
Caelo	Sodium citrate	16095707	9
Caelo	Sodium citrate	1610016-01	4
Caelo	Sodium citrate	16217901	1
Caelo	Sodium citrate	16217902	1
Caelo	Sodium citrate	16217905	18
Caelo	Sodium citrate	16217906	1
Caelo	Sodium citrate	16217908	1
Caelo	Sodium citrate	16217909	10
Caelo	Sodium citrate	16217912	5
Caelo	Sodium citrate	16217913	1
Caelo	Sodium citrate	16217914	5
Caelo	Sodium citrate	16217915	2
Caelo	Sodium citrate	16F10-B01-326093	1
Caelo	Sodium citrate	16F10-B01-327510	1
Caelo	Sodium citrate	170102901	1
Caelo	Sodium citrate	1701029-01	5
Caelo	Sodium citrate	17081501	1
Caelo	Sodium citrate	1710006-02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sodium citrate	171006-02	1
Caelo	Sodium citrate	171025NC/16217909	1
Caelo	Sodium citrate	17323601	34
Caelo	Sodium citrate	17323602	7
Caelo	Sodium citrate	17323603	6
Caelo	Sodium citrate	17323608	39
Caelo	Sodium citrate	17323609	8
Caelo	Sodium citrate	1732361	1
Caelo	Sodium citrate	17323612	5
Caelo	Sodium citrate	1732601	1
Caelo	Sodium citrate	1732608	1
Caelo	Sodium citrate	1792380	1
Caelo	Sodium citrate	17H7-B04-345098	1
Caelo	Sodium citrate	18028305	1
Caelo	Sodium citrate	1807035-01	2
Caelo	Sodium citrate	1807035-02	2
Caelo	Sodium citrate	1807053-01	1
Caelo	Sodium citrate	18208302	22
Caelo	Sodium citrate	18208303	8
Caelo	Sodium citrate	18208305	1
Caelo	Sodium citrate	18208307	23
Caelo	Sodium citrate	18208308	4
Caelo	Sodium citrate	18208313	8
Caelo	Sodium citrate	18208314	3
Caelo	Sodium citrate	18208315	32
Caelo	Sodium citrate	18G25-B07-352737	1
Caelo	Sodium citrate	1901035-01	3
Caelo	Sodium citrate	190890002	11
Caelo	Sodium citrate	190890003	2
Caelo	Sodium citrate	190890004	3
Caelo	Sodium citrate	190890005	3
Caelo	Sodium citrate	190890007	19
Caelo	Sodium citrate	190890009	28
Caelo	Sodium citrate	19089001	4
Caelo	Sodium citrate	19089002	6
Caelo	Sodium citrate	19089003	11
Caelo	Sodium citrate	19089004	32
Caelo	Sodium citrate	1909020-01	1
Caelo	Sodium citrate	19121802	1
Caelo	Sodium citrate	20002150001	2
Caelo	Sodium citrate	20002150003	4
Caelo	Sodium citrate	20004144004	1
Caelo	Sodium citrate	20004144005	3
Caelo	Sodium citrate	20004144008	1
Caelo	Sodium citrate	20004144010	1
Caelo	Sodium citrate	2016-01-28AVIGr	1
Caelo	Sodium citrate	20170412	1
Caelo	Sodium citrate	2019Q-01900	1
Caelo	Sodium citrate	21002580003	4
Caelo	Sodium citrate	21002580004	6
Caelo	Sodium citrate	21002580007	4
Caelo	Sodium citrate	21002580008	2
Caelo	Sodium citrate	21002580009	2
Caelo	Sodium citrate	21002580010	2
Caelo	Sodium citrate	21002580011	2
Caelo	Sodium citrate	21002580012	12
Caelo	Sodium citrate	21002580013	1
Caelo	Sodium citrate	21002580015	1
Caelo	Sodium citrate	21002580016	8
Caelo	Sodium citrate	21002580018	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sodium citrate	21002580019	1
Caelo	Sodium citrate	2101007-01	3
Caelo	Sodium citrate	21121203	1
Caelo	Sodium citrate	2116A-01900	1
Caelo	Sodium citrate	22002778002	1
Caelo	Sodium citrate	22002778003	6
Caelo	Sodium citrate	22002778007	8
Caelo	Sodium citrate	220516(190890009)	1
Caelo	Sodium citrate	220914PML01	1
Caelo	Sodium citrate	23003487003	1
Caelo	Sodium citrate	2345678	1
Caelo	Sodium citrate	2413A-01900	1
Caelo	Sodium citrate	25383143	1
Caelo	Sodium citrate	2543	1
Caelo	Sodium citrate	2815A-01900	1
Caelo	Sodium citrate	2818A-01900	1
Caelo	Sodium citrate	2908022-01	1
Caelo	Sodium citrate	30081802	1
Caelo	Sodium citrate	3040611	1
Caelo	Sodium citrate	4111Q-01900	1
Caelo	Sodium citrate	459842	1
Caelo	Sodium citrate	4680	1
Caelo	Sodium citrate	49131-01900	1
Caelo	Sodium citrate	50815PMS01	1
Caelo	Sodium citrate	516-01900	1
Caelo	Sodium citrate	70214PJK01	1
Caelo	Sodium citrate	8/AKD41	1
Caelo	Sodium citrate	AM1007248703	1
Caelo	Sodium citrate	K-280313-1	1
Caelo	Sodium citrate	P-07081921/18208313	1
Caelo	Sodium citrate	Test	3
Caelo	Sodium citrate	Test123	1
Caelo	Sodium citrate	test13	1
Caelo	Sodium citrate	Testmessung	1
Caelo	Sodium citrate	TestmessungnachRep	1
Caelo	Sodium citrate	Validierungsmessung	1
caeo	Sodium citrate	22002778003	1
Caesar & Loretz / Sa…	Sodium citrate	190890007	1
Caesar & Loretz GmbH…	Sodium citrate	14369406	1
Caesar & Loretz GmbH…	Sodium citrate	20004144005	1
Caesar & Loretz GmbH…	Sodium citrate	21002580003	1
Caesar & Loretz GmbH…	Sodium citrate	18208302	2
Caesar & Loretz GmbH…	Sodium citrate	20002150001	1
Caesar & Loretz GmbH…	Sodium citrate	190890002	1
Caesar & Loretz GmbH /AHD	Sodium citrate	22002778007	1
Caesar & Loretz GmbH/ AHD	Sodium citrate	18208315	1
Caesar & Loretz GmbH…	Sodium citrate	190890007	1
Caesar & Loretz GmbH…	Sodium citrate	19089003	1
Caesar & Loretz GmbH/Gehe	Sodium citrate	18208302	1
Caesar & Loretz GmbH/Gehe	Sodium citrate	18208315	1
Caesar & Loretz GmbH/Gehe	Sodium citrate	21002580003	1
Caesar & Loretz GmbH…	Sodium citrate	190890009	1
Caesar & Loretz GmbH/K	Sodium citrate	190890009	1
Caesar & Loretz GmbH…	Sodium citrate	18208307	1
Caesar & Loretz GmbH…	Sodium citrate	190890009	1
Caesar & Loretz GmbH…	Sodium citrate	19089002	1
Caesar & Loretz GmbH…	Sodium citrate	22002778003	1
Caesar & Loretz GmbH…	Sodium citrate	1701029-01	1
Caesar & Loretz GmbH…	Sodium citrate	18208315	2
Caesar & Loretz GmbH…	Sodium citrate	190890009	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Sodium citrate	19089004	2
Caesar & Loretz GmbH	Sodium citrate	13089334	1
Caesar & Loretz GmbH	Sodium citrate	14112517	1
Caesar & Loretz GmbH	Sodium citrate	14369406	1
Caesar & Loretz GmbH	Sodium citrate	1607040-01	1
Caesar & Loretz GmbH	Sodium citrate	17323601	1
Caesar & Loretz GmbH	Sodium citrate	17323608	1
Caesar & Loretz GmbH	Sodium citrate	18208302	4
Caesar & Loretz GmbH	Sodium citrate	18208305	1
Caesar & Loretz GmbH	Sodium citrate	18208307	4
Caesar & Loretz GmbH	Sodium citrate	18208308	1
Caesar & Loretz GmbH	Sodium citrate	18208315	5
Caesar & Loretz GmbH	Sodium citrate	190890002	3
Caesar & Loretz GmbH	Sodium citrate	190890003	3
Caesar & Loretz GmbH	Sodium citrate	190890004	4
Caesar & Loretz GmbH	Sodium citrate	190890007	8
Caesar & Loretz GmbH	Sodium citrate	190890009	9
Caesar & Loretz GmbH	Sodium citrate	19089002	2
Caesar & Loretz GmbH	Sodium citrate	19089003	3
Caesar & Loretz GmbH	Sodium citrate	19089004	7
Caesar & Loretz GmbH	Sodium citrate	1909020-01	1
Caesar & Loretz GmbH	Sodium citrate	20002150003	4
Caesar & Loretz GmbH	Sodium citrate	21002580004	1
Caesar & Loretz GmbH	Sodium citrate	21002580007	1
Caesar & Loretz GmbH	Sodium citrate	21002580009	2
Caesar & Loretz GmbH	Sodium citrate	2100258001	1
Caesar & Loretz GmbH	Sodium citrate	21002580010	1
Caesar & Loretz GmbH	Sodium citrate	21002580011	3
Caesar & Loretz GmbH	Sodium citrate	21002580012	3
Caesar & Loretz GmbH	Sodium citrate	22002778003	1
Caesar & Loretz/Geil...	Sodium citrate	190890007	1
Caesar&Loretz GmbH/Anzag	Sodium citrate	14369407	1
Caesar&Loretz GmbH	Sodium citrate	12045026	1
Caesar&Loretz GmbH	Sodium citrate	14112502	1
Caesar/Noweda	Sodium citrate	12045008	1
Caeser und Loretz GmbH	Sodium citrate	18208308	1
Caleo	Sodium citrate	18208302	1
Calo, Hilden/ Phönix	Sodium citrate	19089004	1
Cealo/Sanacorp	Sodium citrate	21002580012	1
Cealo	Sodium citrate	190890007	1
Defektur	Sodium citrate	19121902	1
Delta Apotheke	Sodium citrate	17323608	1
Eigenherstellung Defektur	Sodium citrate	5082103	1
Eigenherstellung/ De...	Sodium citrate	12102101	1
EuRho / Alliance	Sodium citrate	1807035-02	1
EuRho / Noweda	Sodium citrate	1807035-01	1
EuRho / Phoenix	Sodium citrate	151101017-01	1
EuRho/ AHD	Sodium citrate	1701029-01	1
EuRho/ Phönix	Sodium citrate	3048768	1
EuRho/Gehe	Sodium citrate	1901035-01	2
EuRho/Jenne	Sodium citrate	1909020-01	1
EuRho/Noweda	Sodium citrate	2206011-01	1
EuRho/Sanacorp	Sodium citrate	1107011-02	1
EuRho/Sanacorp	Sodium citrate	1506041-01	1
EuRho	Sodium citrate	1070102901	1
EuRho	Sodium citrate	1107011-02	1
EuRho	Sodium citrate	1205026-02	1
EuRho	Sodium citrate	1211030-01	1
EuRho	Sodium citrate	1311035-01	1
EuRho	Sodium citrate	140403301	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho	Sodium citrate	1404033-01	2
EuRho	Sodium citrate	1412014-01	1
EuRho	Sodium citrate	1607040-01	5
EuRho	Sodium citrate	1901035-01	1
Eurho	Sodium citrate	2007022-01	1
EuRho	Sodium citrate	2007022-01	1
Eurho	Sodium citrate	2101007-01	1
EuRho	Sodium citrate	3032981	1
EuRho	Sodium citrate	3108854	1
EuRho	Sodium citrate	4611M-01900	1
Euro Gehe	Sodium citrate	1909020-01	1
Euro OTC	Sodium citrate		5
Euro OTC	Sodium citrate	100800903	1
Euro OTC	Sodium citrate	1017I-01900	1
Euro OTC	Sodium citrate	1073240	1
Euro OTC	Sodium citrate	1107011-01	1
Euro OTC	Sodium citrate	1107011-02	1
Euro OTC	Sodium citrate	1205026-02	4
Euro OTC	Sodium citrate	1211030-01	10
Euro OTC	Sodium citrate	12345	2
Euro OTC	Sodium citrate	1305001-01	11
Euro OTC	Sodium citrate	1311025-01	1
Euro OTC	Sodium citrate	1311035-01	27
Euro OTC	Sodium citrate	13I24-B13-287921	1
Euro OTC	Sodium citrate	140403301	5
Euro OTC	Sodium citrate	1404033-01	13
Euro OTC	Sodium citrate	1412014-01	18
Euro OTC	Sodium citrate	1413M-01900	1
Euro OTC	Sodium citrate	14201401	1
Euro OTC	Sodium citrate	1506041-01	18
Euro OTC	Sodium citrate	150922-1078	1
Euro OTC	Sodium citrate	151101701	3
Euro OTC	Sodium citrate	1511017-01	32
Euro OTC	Sodium citrate	15111017-01	1
Euro OTC	Sodium citrate	1521017-01	1
Euro OTC	Sodium citrate	15212705	1
Euro OTC	Sodium citrate	156422	1
Euro OTC	Sodium citrate	16070-01	1
Euro OTC	Sodium citrate	1607040-01	20
Euro OTC	Sodium citrate	160740-01	1
Euro OTC	Sodium citrate	161001601	1
Euro OTC	Sodium citrate	1610016-01	45
Euro OTC	Sodium citrate	1610016601	1
Euro OTC	Sodium citrate	1645265	3
Euro OTC	Sodium citrate	17010006-02	1
Euro OTC	Sodium citrate	170102901	1
Euro OTC	Sodium citrate	1701029-01	43
Euro OTC	Sodium citrate	1701029-02	1
Euro OTC	Sodium citrate	17061407	1
Euro OTC	Sodium citrate	1710006-01	12
Euro OTC	Sodium citrate	1710006-015607	1
Euro OTC	Sodium citrate	1710006-02	10
Euro OTC	Sodium citrate	171006-02	1
Euro OTC	Sodium citrate	180703501	1
Euro OTC	Sodium citrate	1807035-01	36
Euro OTC	Sodium citrate	1807035-01ciclo	1
Euro OTC	Sodium citrate	1807035-02	10
Euro OTC	Sodium citrate	180735-01	1
Euro OTC	Sodium citrate	1819A-01900	1
Euro OTC	Sodium citrate	187035-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Sodium citrate	19009020-01	1
Euro OTC	Sodium citrate	190103501	1
Euro OTC	Sodium citrate	1901035-01	52
Euro OTC	Sodium citrate	19090120-01	1
Euro OTC	Sodium citrate	1909020	1
Euro OTC	Sodium citrate	1909020-01	38
Euro OTC	Sodium citrate	190902-01	1
Euro OTC	Sodium citrate	190920	1
Euro OTC	Sodium citrate	2002040-01	30
Euro OTC	Sodium citrate	2002040-1	1
Euro OTC	Sodium citrate	200702201	1
Euro OTC	Sodium citrate	2007022-01	37
Euro OTC	Sodium citrate	20200810-6	1
Euro OTC	Sodium citrate	20A20-F03-369331	1
Euro OTC	Sodium citrate	2101007	2
Euro OTC	Sodium citrate	210100701	1
Euro OTC	Sodium citrate	2101007-01	44
Euro OTC	Sodium citrate	2114M1900	1
Euro OTC	Sodium citrate	2206011-01	30
Euro OTC	Sodium citrate	22101305	1
Euro OTC	Sodium citrate	2212001-01	1
Euro OTC	Sodium citrate	22606011-01	1
Euro OTC	Sodium citrate	23062015C	1
Euro OTC	Sodium citrate	25425	2
Euro OTC	Sodium citrate	2546426	1
Euro OTC	Sodium citrate	2903001-01	1
Euro OTC	Sodium citrate	30111301	1
Euro OTC	Sodium citrate	3021717	1
Euro OTC	Sodium citrate	3032805	3
Euro OTC	Sodium citrate	3032981	1
Euro OTC	Sodium citrate	3048768	3
Euro OTC	Sodium citrate	30611044	5
Euro OTC	Sodium citrate	3065202	2
Euro OTC	Sodium citrate	3087522	2
Euro OTC	Sodium citrate	3095222	3
Euro OTC	Sodium citrate	3108854	1
Euro OTC	Sodium citrate	3454	1
Euro OTC	Sodium citrate	345678	1
Euro OTC	Sodium citrate	358528	1
Euro OTC	Sodium citrate	4716E-01900	1
Euro OTC	Sodium citrate	48(08598497)	1
Euro OTC	Sodium citrate	5116E-01900	1
Euro OTC	Sodium citrate	815757/6745	1
Euro OTC	Sodium citrate	901035-011	1
euro//Noweda	Sodium citrate	1701029-01	1
Euro/Phönix	Sodium citrate	1305001-01	1
Euro/Phönix	Sodium citrate	1610016-01	1
Euro	Sodium citrate	1815M-01900	1
Europ Ots Pharma	Sodium citrate	13089304	1
Fagron	Sodium citrate	1017Q-01900	1
Fagron	Sodium citrate	1161207	3
Fagron	Sodium citrate	1172108	1
Fagron	Sodium citrate	1176767	3
Fagron	Sodium citrate	1190802	1
Fagron	Sodium citrate	1211142	2
Fagron	Sodium citrate	1219546	2
Fagron	Sodium citrate	1227297	3
Fagron	Sodium citrate	1232850	2
Fagron	Sodium citrate	12339502	1
Fagron	Sodium citrate	1234468	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Sodium citrate	1234567	1
Fagron	Sodium citrate	123456test	1
Fagron	Sodium citrate	1241068	1
Fagron	Sodium citrate	1250221	2
Fagron	Sodium citrate	1262240	4
Fagron	Sodium citrate	12A05-N04	2
Fagron	Sodium citrate	12E04-N05	1
Fagron	Sodium citrate	12I10-N01	1
Fagron	Sodium citrate	12J26-N02	3
Fagron	Sodium citrate	13/24-B13-287921	3
Fagron	Sodium citrate	13089331	1
Fagron	Sodium citrate	13A07-N01	6
Fagron	Sodium citrate	13A07-NO1	1
Fagron	Sodium citrate	13B28-N02	6
Fagron	Sodium citrate	13D09N01	1
Fagron	Sodium citrate	13D09-N01	4
Fagron	Sodium citrate	13I24-B13-287921	2
Fagron	Sodium citrate	13l24-B13	1
Fagron	Sodium citrate	14112502	2
Fagron	Sodium citrate	14369402	2
Fagron	Sodium citrate	14A13_b02_300395	1
Fagron	Sodium citrate	14A13-B02-294541	8
Fagron	Sodium citrate	14A13B02300395	1
Fagron	Sodium citrate	14A13-B02-300395	4
Fagron	Sodium citrate	1511017-01	1
Fagron	Sodium citrate	15C27	1
Fagron	Sodium citrate	15C27-B01-309893	5
Fagron	Sodium citrate	15-C27-B01-309893	1
Fagron	Sodium citrate	15C27-B01-312231	6
Fagron	Sodium citrate	15C27-B01-316106	2
Fagron	Sodium citrate	15c27-b01-321097	1
Fagron	Sodium citrate	15C27B01-321097	1
Fagron	Sodium citrate	15C27-B01-321097	1
Fagron	Sodium citrate	15C27-B01-3211097	1
Fagron	Sodium citrate	15C27-B01-323451	3
Fagron	Sodium citrate	15C27-B01-3234551	1
Fagron	Sodium citrate	160614	1
Fagron	Sodium citrate	16F10-B01-326088	2
Fagron	Sodium citrate	16F10-B01-327510	5
Fagron	Sodium citrate	16F10-B1-327510	1
Fagron	Sodium citrate	1710006-01	1
Fagron	Sodium citrate	179915	3
Fagron	Sodium citrate	179915-0001	2
Fagron	Sodium citrate	17A26-B04-331525	1
Fagron	Sodium citrate	17A26-B04-331528	14
Fagron	Sodium citrate	17A26-B04-332866	1
Fagron	Sodium citrate	17A26-B04-332871	26
Fagron	Sodium citrate	17A26-B04-335680	24
Fagron	Sodium citrate	17A26-B04-335883	2
Fagron	Sodium citrate	17H04-B04-345098	1
Fagron	Sodium citrate	17H07	1
Fagron	Sodium citrate	17H07-B04	2
Fagron	Sodium citrate	17H07-B04_338530	28
Fagron	Sodium citrate	17H07-B04-341746	5
Fagron	Sodium citrate	17H07-B04-345098	2
Fagron	Sodium citrate	1807035-01	1
Fagron	Sodium citrate	18B14-B08	1
Fagron	Sodium citrate	18B14-B08-348067	6
Fagron	Sodium citrate	18C05-B03	2
Fagron	Sodium citrate	18C05-B03350564	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Sodium citrate	18C05-B03-350564	3
Fagron	Sodium citrate	18G25-B07	2
Fagron	Sodium citrate	18G25-B07-352737	4
Fagron	Sodium citrate	18G25-B07-354623	2
Fagron	Sodium citrate	18G25-B07-354812	4
Fagron	Sodium citrate	18L13B023549449	1
Fagron	Sodium citrate	18l13b02359449	1
Fagron	Sodium citrate	18L13-B02-359449	11
Fagron	Sodium citrate	18L13-B02-359451	3
Fagron	Sodium citrate	18L13-Bo2-359449	1
Fagron	Sodium citrate	18L13-BO2-359449	1
Fagron	Sodium citrate	19F19-B01	2
Fagron	Sodium citrate	19F19-B01-363699	2
Fagron	Sodium citrate	19F19-B01-363701	4
Fagron	Sodium citrate	19I26-F01-365434	4
Fagron	Sodium citrate	19I26F01365444	1
Fagron	Sodium citrate	19I26FO1365444	1
Fagron	Sodium citrate	19l26-F01-365434	1
Fagron	Sodium citrate	2007022-01	1
Fagron	Sodium citrate	20A20F03	1
Fagron	Sodium citrate	20A20-F03	4
Fagron	Sodium citrate	20A20-F03-069331	1
Fagron	Sodium citrate	20A20-f03-368130	1
Fagron	Sodium citrate	20A20-F03-368130	11
Fagron	Sodium citrate	20A20-F03-369331	5
Fagron	Sodium citrate	20A20-F03-369333	13
Fagron	Sodium citrate	20B24-F03-374173	1
Fagron	Sodium citrate	20K19-F02	1
Fagron	Sodium citrate	20K19-F02-376135	1
Fagron	Sodium citrate	20K19-F02-376136	2
Fagron	Sodium citrate	22K17-B15-221097	1
Fagron	Sodium citrate	22K17-B15-22197	1
Fagron	Sodium citrate	24121301	1
Fagron	Sodium citrate	2OA2O-FO3-368130	1
Fagron	Sodium citrate	2OA2O-FO3-369331	1
Fagron	Sodium citrate	2OAO-FO3-368130	1
Fagron	Sodium citrate	2OB24-FO3374173	1
Fagron	Sodium citrate	306084	1
Fagron	Sodium citrate	31051202	1
Fagron	Sodium citrate	3311E-01900	1
Fagron	Sodium citrate	712A-01900	1
Fagron	Sodium citrate	801-3636909	1
Fagron	Sodium citrate	815Q-01900	1
Fagron	Sodium citrate	F03-368130	1
Fagron	Sodium citrate	F03-3681300	1
Fagron	Sodium citrate	F0336813000	1
Fagron	Sodium citrate	F03-3693301	1
Fagron	Sodium citrate	Probe	1
Fargo/Phoenix	Sodium citrate	1511017-01	1
Fargon GmbH & Co.KG	Sodium citrate	16F10-B01-326088	1
Fargon/Alliance HC	Sodium citrate	13/24-B13-287921	1
fargon	Sodium citrate	100772-114-91	1
Fiebig	Sodium citrate	12J26-NO2	1
Fiebig	Sodium citrate	1607002-01	2
Fiebig	Sodium citrate	1610016-01	1
Fiebig	Sodium citrate	190890002	1
Fragon	Sodium citrate	18L13-BO2-359449	1
Gatt-Koller	Sodium citrate	1073/04121412	1
Gehe 26.05.2014	Sodium citrate	13B28-N02	1
Gehe amax	Sodium citrate	1610016-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe Rostock	Sodium citrate	2002040-01	1
Gehe/Euro	Sodium citrate	1404033-01	2
Gehe/Euro	Sodium citrate	1412014-01	6
Gehe	Sodium citrate	12045026	1
Gehe	Sodium citrate	1311035-01	1
Gehe	Sodium citrate	14369413	2
GEHE	Sodium citrate	1607040-01	2
GEHE	Sodium citrate	1710006-02	1
GEHE	Sodium citrate	17A26-B04-331525	6
GEHE	Sodium citrate	17A26-B04-332866	5
GEHE	Sodium citrate	17H507-A04-347340	1
Gehe	Sodium citrate	18B14-B08-348067	1
Gehe	Sodium citrate	18G25-B07	1
gehe	Sodium citrate	18G25-B07-354812	1
Gehe	Sodium citrate	18L13-B02-359449	1
Gehe	Sodium citrate	1901035-01	3
Gehe	Sodium citrate	19089003	1
Gehe	Sodium citrate	2007022-01	1
GEHE	Sodium citrate	21002580016	1
Gehe	Sodium citrate	2101007-01	1
Gehe	Sodium citrate	22002778007	2
Gehe	Sodium citrate	2206011-01	1
Gehe	Sodium citrate	2212001-01	2
GEHE	Sodium citrate	2212001-01	1
Hageda	Sodium citrate	2002040-01	1
HiperScan	Sodium citrate		1
Jenne	Sodium citrate	21002580007	1
Jungbunzlauer/Phoenix	Sodium citrate	20A20-F03	1
Kehr	Sodium citrate	17A26-B04-331525	1
Kehr	Sodium citrate	23000473002	1
L12	Sodium citrate	16217905	1
L12	Sodium citrate	17323608	1
Merck	Sodium citrate		2
Merck	Sodium citrate	37/17	1
Merck	Sodium citrate	AM0602648542	1
Merck	Sodium citrate	AM1005848809	1
Merck	Sodium citrate	AM1171048839	1
Merck	Sodium citrate	AM1171148726	1
Merk	Sodium citrate	AM0602648	1
Nachprüfung 31.12.2018	Sodium citrate	14112517	2
Nachprüfung	Sodium citrate	1205026-02	1
Noweda	Sodium citrate	11127001	1
Noweda	Sodium citrate	12045026	1
Noweda	Sodium citrate	14A13-B02-294541	1
Noweda	Sodium citrate	1511017-01	1
Noweda	Sodium citrate	16095707	1
Noweda	Sodium citrate	1701029-01	1
Noweda	Sodium citrate	1710006-01	1
Noweda	Sodium citrate	17H07-B04	1
Noweda	Sodium citrate	17H07-B04-341746	1
Noweda	Sodium citrate	17H07-B04-345098	1
Noweda	Sodium citrate	18208315	2
Noweda	Sodium citrate	1901035-01	1
Noweda	Sodium citrate	1909020-01	1
Noweda	Sodium citrate	19F19-B01-363699	1
Noweda	Sodium citrate	22002778007	3
Noweda	Sodium citrate	2202778003	1
Noweda	Sodium citrate	2212001-02	1
Noweda	Sodium citrate	22K17-B15-221097	1
Noweda	Sodium citrate	3032981	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Nowedan 15.11.2019	Sodium citrate	1909020-01	1
Phoenix /Fargon	Sodium citrate	20A20-F03-368130	1
Phoenix 30.05.2016	Sodium citrate	14369423	1
Phoenix/Noweda	Sodium citrate	1506041-01	2
Phoenix	Sodium citrate	1506041-01	1
Phoenix	Sodium citrate	1511017-01	2
Phoenix	Sodium citrate	1710006-02	1
Phoenix	Sodium citrate	1901035-01	2
Phoenix	Sodium citrate	191291911	1
Phoenix	Sodium citrate	20a20-f03-368130	1
Phoenix	Sodium citrate	22002778007	1
Phoenix	Sodium citrate	2212001-01	1
Phoenix	Sodium citrate	3422	1
Phönix	Sodium citrate	12045019	1
Phönix	Sodium citrate	12045024	1
Phönix	Sodium citrate	1205026-02	1
Phönix	Sodium citrate	1807035-01	2
Phönix	Sodium citrate	1807035-02	1
Phönix	Sodium citrate	190890007	1
Phönix	Sodium citrate	21002580012	1
Phönix	Sodium citrate	22002778003	3
Phönix	Sodium citrate	22002778007	2
Phönix	Sodium citrate	22K17-B15-223095	1
Retest	Sodium citrate	1610016-01	1
Röntgen	Sodium citrate	17323601	1
Sanacoro W.E:15.05.1...	Sodium citrate	14112502	1
Sanacorp	Sodium citrate	13089308	1
Sanacorp	Sodium citrate	13089331	1
Sanacorp	Sodium citrate	1311035-01	1
Sanacorp	Sodium citrate	1436407	1
Sanacorp	Sodium citrate	17A26-B04-332866	1
Sanacorp	Sodium citrate	190890007	1
Sanacorp	Sodium citrate	21002580012	1
Sanacorp	Sodium citrate	21002580013	1
Sanacorp	Sodium citrate	2101007-01	1
Sanacorp	Sodium citrate	22002778007	1
Sanacorp	Sodium citrate	2206011-01	1
Sanacorp	Sodium citrate	2212001-01	1
Sanacorp	Sodium citrate	23003487003	1
Sanacorp	Sodium citrate	EuRho	1
Test	Sodium citrate		1
TEST	Sodium citrate		1
Test	Sodium citrate	1234	1
Test	Sodium citrate	12345	1
Test	Sodium citrate	123456	1
Unisan	Sodium citrate	1701029-01	1
Unisan	Sodium citrate	S/WReferenzUmstell	1
VDL;16.05.15;3,83EUR	Sodium citrate	14369406	1
wepa	Sodium citrate	1909020-01	1

- 233 819 spectra from 1513 *Apo-Ident* customers from a total of 48 855 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sodium citrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sodium citrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	540	0	152 422
Type B	0	810	0	201 274
Type C	0	2120	128	233 819

The substance/substance group *Sodium citrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8889 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2593 %)
Type C	100.0000 % (> 99.9007 %)	94.3060 % (> 94.1726 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20662	21839	6.84	137.95
20918	21670	8.62	138.21
21670	21670	0.00	136.73
21718	21670	4.04	135.97
21778	21670	5.55	137.64
21839	21839	0.00	139.28
21997	21997	0.00	140.14
22843	21997	9.04	143.22
22859	22859	0.00	147.85
22996	22996	0.00	140.40
25324	25324	0.00	143.35

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sodium cromoglicate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20775-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium cromoglicate; Cromolyn sodium; Natrii cromoglicas

Special notes

When selecting the *Sodium cromoglicate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sodium cromoglicate	11	12	14

Second-stage model

For differentiation of the substance/substance group *Sodium cromoglicate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sodium cromoglicate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Oxytetracycline hydrochloride	97.55	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sodium cromoglicate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sodium cromoglicate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium cromoglicate	11114501	20776	80	20110518
Caelo	Sodium cromoglicate	13232802	21375	20	1505352
Caelo	Sodium cromoglicate	13232802	21376	110	20130905
Caelo	Sodium cromoglicate	15224404	21990	60	20150625
Caelo	Sodium cromoglicate	20003498	25641	40	20201120*
Euro OTC	Sodium cromoglicate	1403017-01	21981	60	20140505
Euro OTC	Sodium cromoglicate	1510018	22231	60	20151109*
Euro OTC	Sodium cromoglicate	1703027	23383	40	20170405*
Euro OTC	Sodium cromoglicate	2012005	25570	40	20210115*
Euro OTC	Sodium cromoglicate	2407017	27366	40	20240814*
Fagron	Sodium cromoglicate	12C09-N02	20775	79	1401553
Fagron	Sodium cromoglicate	13G24-N04	21260	40	20130515

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 669 spectra of 12 reference samples from the substance/substance group *Sodium cromoglicate*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 293 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 530 spectra of 15 reference samples from the substance/substance group *Sodium cromoglicate*.

- Among them are spectra of independent samples from 12 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium cromoglicate	173081	23855	30
Caelo	Sodium cromoglicate	182657	24382	40
Euro OTC	Sodium cromoglicate	1112003-01	20778	40
Euro OTC	Sodium cromoglicate	1711024	23871	40
Euro OTC	Sodium cromoglicate	1811016	24424	40
Euro OTC	Sodium cromoglicate	2004037	25268	40
Euro OTC	Sodium cromoglicate	2007031	25454	40
Euro OTC	Sodium cromoglicate	2211013	26432	40
Euro OTC	Sodium cromoglicate	2306002	26767	40
Euro OTC	Sodium cromoglicate	2306008	26768	40
Fagron	Sodium cromoglicate	15C23-B01-307751	22972	40
Fagron	Sodium cromoglicate	23A04-B02-224458	26608	40
Euro OTC	Sodium cromoglicate	2211013	26432SI	20
Euro OTC	Sodium cromoglicate	2306002	26767SI	20
Fagron	Sodium cromoglicate	23A04-B02-224458	26608SI	20

- 201 554 spectra from a total of 4033 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 27 spectra from 19 *Apo-Ident* customers from 17 batches from the substance/substance group *Sodium cromoglicate*.
- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Bombastus	Sodium cromoglicate	15414502	1
Caelo	Sodium cromoglicate	12301102	1
Caelo	Sodium cromoglicate	15224404	1
Caelo	Sodium cromoglicate	16270705	3
Caelo	Sodium cromoglicate	17308104	1
Caelo	Sodium cromoglicate	18265707	1
Caelo	Sodium cromoglicate	20003498009	1
Caelo	Sodium cromoglicate	20003499001	2
Caelo	Sodium cromoglicate	5113A-02831	1
Caesar & Loretz GmbH...	Sodium cromoglicate	18265704	2
Caesar & Loretz GmbH	Sodium cromoglicate	18265706	5
E Plus	Sodium cromoglicate	15414502	1
Euro OTC	Sodium cromoglicate	1403017-01	1
Euro OTC	Sodium cromoglicate	1510018-01	1
Euro OTC	Sodium cromoglicate	170302701	1
Euro OTC	Sodium cromoglicate	1850002692	1
Fagron	Sodium cromoglicate	13E22-N11	1
Fagron	Sodium cromoglicate	13G24-N04	1
Sanacorp	Sodium cromoglicate	20003499001	1

- 236 040 spectra from 1515 *Apo-Ident* customers from a total of 49 241 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sodium cromoglicate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sodium cromoglicate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	668	1	152 293
Type B	0	530	0	201 554
Type C	0	27	0	236 040

The substance/substance group *Sodium cromoglicate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	99.8505 % (> 99.4021 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.8679 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 77.7778 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20775	20775	0.00	235.87
20776	22231	42.22	237.96
21260	22231	15.10	229.93
21375	21375	0.00	299.04
21376	21375	22.94	254.71
21981	22231	26.22	203.86
21990	22231	23.06	219.84
22231	22231	0.00	219.18
23383	23383	0.00	216.57
25570	25570	0.00	225.26
25641	25641	0.00	225.96
27366	27366	0.00	320.99

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sodium cyclamate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20917-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium cyclamate; Natrii cyclamas

Special notes

When selecting the *Sodium cyclamate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sodium cyclamate	6	3	40

Second-stage model

For differentiation of the substance/substance group *Sodium cyclamate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sodium cyclamate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Menthol	114.46	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sodium cyclamate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sodium cyclamate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium cyclamate	12256803	20917	40	1401418
Caelo	Sodium cyclamate	12105622	21380	40	20120423
Caelo	Sodium cyclamate	182167	24379	40	20181023*
Caelo	Sodium cyclamate	20004287009	26234	40	20201216
Caelo	Sodium cyclamate	20004287009	26234SI	20	20201216
Caelo	Sodium cyclamate	24002330	27429	40	20241028*
Gatt-Koller	Sodium cyclamate	23J00242	26702	40	20230308
Gatt-Koller	Sodium cyclamate	23J00242	26702SI	20	20230308

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 280 spectra of 8 reference samples from the substance/substance group *Sodium cyclamate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 682 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Sodium cyclamate*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium cyclamate	16119302	23259	40
Caelo	Sodium cyclamate	170411	23853	40
Caelo	Sodium cyclamate	22003585	26716	40
Caelo	Sodium cyclamate	22003585	26716SI	20

- 201 944 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 223 spectra from 178 *Apo-Ident* customers from 42 batches from the substance/substance group *Sodium cyclamate*.

- Among them are spectra of independent samples from 40 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sodium cyclamate	20004287013	1
	Sodium cyclamate	20004287014	1
	Sodium cyclamate	20004287017	3
	Sodium cyclamate	22003585002	3
	Sodium cyclamate	22003585006	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sodium cyclamate	10380915	2
Caelo	Sodium cyclamate	11204205	1
Caelo	Sodium cyclamate	14149602	1
Caelo	Sodium cyclamate	15201601	2
Caelo	Sodium cyclamate	15201606	2
Caelo	Sodium cyclamate	15201608	4
Caelo	Sodium cyclamate	15201614	1
Caelo	Sodium cyclamate	16119302	4
Caelo	Sodium cyclamate	16119302/2280217	1
Caelo	Sodium cyclamate	16119308	8
Caelo	Sodium cyclamate	16119310	1
Caelo	Sodium cyclamate	17041102	8
Caelo	Sodium cyclamate	17362202	7
Caelo	Sodium cyclamate	17362203	1
Caelo	Sodium cyclamate	17362207	8
Caelo	Sodium cyclamate	17362208	8
Caelo	Sodium cyclamate	179617362207	1
Caelo	Sodium cyclamate	17961821675	1
Caelo	Sodium cyclamate	18053101	1
Caelo	Sodium cyclamate	182167002	6
Caelo	Sodium cyclamate	182167004	6
Caelo	Sodium cyclamate	182167005	6
Caelo	Sodium cyclamate	18216702	9
Caelo	Sodium cyclamate	18216704	7
Caelo	Sodium cyclamate	18216707	19
Caelo	Sodium cyclamate	200004287003	1
Caelo	Sodium cyclamate	20004278013	1
Caelo	Sodium cyclamate	20004285001	7
Caelo	Sodium cyclamate	20004287003	3
Caelo	Sodium cyclamate	20004287005	6
Caelo	Sodium cyclamate	20004287007	7
Caelo	Sodium cyclamate	20004287009	8
Caelo	Sodium cyclamate	20004287011	4
Caelo	Sodium cyclamate	20004287013	3
Caelo	Sodium cyclamate	20004287014	4
Caelo	Sodium cyclamate	200042887005	1
Caelo	Sodium cyclamate	22003585002	2
Caelo	Sodium cyclamate	3092002	1
Caeol/ Noweda	Sodium cyclamate	16119302	1
Caesar & Loretz GmbH...	Sodium cyclamate	20004287013	1
Caesar & Loretz GmbH...	Sodium cyclamate	18216704	1
Caesar & Loretz GmbH...	Sodium cyclamate	182167004	2
Caesar & Loretz GmbH/AHD	Sodium cyclamate	20004287013	1
Caesar & Loretz GmbH...	Sodium cyclamate	182167005	1
Caesar & Loretz GmbH/Gehe	Sodium cyclamate	20004285001	3
Caesar & Loretz GmbH...	Sodium cyclamate	20004287003	1
Caesar & Loretz GmbH...	Sodium cyclamate	20004287007	1
Caesar & Loretz GmbH...	Sodium cyclamate	20004287014	1
Caesar & Loretz GmbH...	Sodium cyclamate	20004287007	1
Caesar & Loretz GmbH	Sodium cyclamate	12105622	1
Caesar & Loretz GmbH	Sodium cyclamate	17362208	3
Caesar & Loretz GmbH	Sodium cyclamate	182167002	3
Caesar & Loretz GmbH	Sodium cyclamate	182167004	4
Caesar & Loretz GmbH	Sodium cyclamate	182167005	4
Caesar & Loretz GmbH	Sodium cyclamate	18216702	3
Caesar & Loretz GmbH	Sodium cyclamate	18216707	4
Caesar & Loretz GmbH	Sodium cyclamate	20004285001	2
Caesar & Loretz GmbH	Sodium cyclamate	20004287003	3
Caesar & Loretz GmbH	Sodium cyclamate	20004287013	1
Caesar & Loretz GmbH	Sodium cyclamate	20004287014	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar&Loretz GmbH/ …	Sodium cyclamate	16119308	1
Euro OTC	Sodium cyclamate	16119302	1
Phoenix	Sodium cyclamate	20004287014	1
Phoenix	Sodium cyclamate	22003585002	1
Phoenix	Sodium cyclamate	787/03100611	1
Phönix	Sodium cyclamate	182167002	1

- 235 844 spectra from 1515 *Apo-Ident* customers from a total of 49 217 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sodium cyclamate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sodium cyclamate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	140	0	201 944
Type C	0	222	1	235 844

The substance/substance group *Sodium cyclamate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	99.5516 % (> 98.2063 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20917	20917	0.00	181.62
21380	20917	17.26	179.20
24379	24379	0.00	184.01
26234	24379	11.94	183.27
26702	27429	47.44	180.26
27429	27429	0.00	184.12

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sodium dihydrogen phosphate dihydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10005937-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium dihydrogen phosphate dihydrate; Natrii dihydrogenophosphas dihydricus

Special notes

When selecting the *Sodium dihydrogen phosphate dihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sodium dihydrogen phosphate dihydrate	4	3	10

Second-stage model

For differentiation of the substance/substance group *Sodium dihydrogen phosphate dihydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sodium dihydrogen phosphate dihydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	73.79	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sodium dihydrogen phosphate dihydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sodium dihydrogen phosphate dihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium dihydrogen phospha…	22001753	26560	40	20220706*
Caelo	Sodium dihydrogen phospha…	22001753	26560SI	20	20220706*
Caelo	Sodium dihydrogen phospha…	24001049	27310	30	20240502*
Euro OTC	Sodium dihydrogen phospha…	2106004	25786	50	20210624*
Euro OTC	Sodium dihydrogen phospha…	2204005	26101	40	20220517*
Euro OTC	Sodium dihydrogen phospha…	2204005	26101SI	20	20220517*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 6 reference samples from the substance/substance group *Sodium dihydrogen*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

phosphate dihydrate. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 152 762 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 4 reference samples from the substance/substance group *Sodium dihydrogen phosphate dihydrate*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium dihydrogen phospha…	21001537	25802	50
Euro OTC	Sodium dihydrogen phospha…	2109011	25817	50
Euro OTC	Sodium dihydrogen phospha…	2307018	26860	40
Euro OTC	Sodium dihydrogen phospha…	2307018	26860SI	20

- 201 924 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 16 spectra from 16 *Apo-Ident* customers from 10 batches from the substance/substance group *Sodium dihydrogen phosphate dihydrate*.

- Among them are spectra of independent samples from 10 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sodium dihydrogen phospha…	22001753006	2
	Sodium dihydrogen phospha…	22001753011	2
	Sodium dihydrogen phospha…	2204005-01	1
Caelo	Sodium dihydrogen phospha…	12198506	1
Caelo	Sodium dihydrogen phospha…	12198510	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sodium dihydrogen phospha…	12198517	2
Caelo	Sodium dihydrogen phospha…	13D08-N25	1
Euro OTC	Sodium dihydrogen phospha…	1209004-01	2
Euro OTC	Sodium dihydrogen phospha…	1305028-01	2
Fagron	Sodium dihydrogen phospha…	12L05-N05	1
Gehe	Sodium dihydrogen phospha…	12198510	1

- 236 051 spectra from 1515 *Apo-Ident* customers from a total of 49 248 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sodium dihydrogen phosphate dihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sodium dihydrogen phosphate dihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	160	0	201 924
Type C	0	16	0	236 051

The substance/substance group *Sodium dihydrogen phosphate dihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25786	25786	0.00	97.92
26101	26101	0.00	58.31
26560	26560	0.00	55.78
27310	27310	0.00	53.33

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sodium edetate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20937-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium edetate; Dinatrii edetas

Special notes

When selecting the *Sodium edetate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sodium edetate	7	17	236

Second-stage model

For differentiation of the substance/substance group *Sodium edetate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sodium edetate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prednisolon dihydrogen phosphate di…	97.73	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sodium edetate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sodium edetate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium edetate	13142009	21362	40	20130524
Caelo	Sodium edetate	161364	22465	60	20160504*
Euro OTC	Sodium edetate	1609023	22915	40	20170106*
Euro OTC	Sodium edetate	1812016	24414	40	20190116*
Fagron	Sodium edetate	13E15-N05	20937	40	1402193
Fagron	Sodium edetate	16F21-B02-325085	22926	40	20160713
Fagron	Sodium edetate	22G15-B01-224176	26394	40	20220803
Fagron	Sodium edetate	22G15-B01-224176	26394SI	20	20220803

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 320 spectra of 8 reference samples from the substance/substance group *Sodium edetate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 642 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 760 spectra of 20 reference samples from the substance/substance group *Sodium edetate*.

- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium edetate	172618	23663	40
Caelo	Sodium edetate	20001878	25209	40
Caelo	Sodium edetate	21001224	25803	40
Caelo	Sodium edetate	22003154	26486	40
Caelo	Sodium edetate	24001067	27329	40
Euro OTC	Sodium edetate	1609023-01	22950	40
Euro OTC	Sodium edetate	1704011	23390	40
Euro OTC	Sodium edetate	1806007	24157	40
Euro OTC	Sodium edetate	1807025	24159	40
Euro OTC	Sodium edetate	1901032	24472	40
Euro OTC	Sodium edetate	1909030	24958	40
Euro OTC	Sodium edetate	2004003	25168	40
Euro OTC	Sodium edetate	2008009	25314	40
Euro OTC	Sodium edetate	2205014	26188	40
Euro OTC	Sodium edetate	2209004	26335	40
Euro OTC	Sodium edetate	2402026	27155	40
Fagron	Sodium edetate	24C25-B37-001217	27380	40
Caelo	Sodium edetate	172618	23818	40
Euro OTC	Sodium edetate	2205014	26188SI	20
Euro OTC	Sodium edetate	2209004	26335SI	20

- 201 324 spectra from a total of 4028 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information

provided by the customer regarding manufacturer and batch number.

- 1044 spectra from 591 *Apo-Ident* customers from 250 batches from the substance/substance group *Sodium edetate*.
- Among them are spectra of independent samples from 236 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sodium edetate		1
	Sodium edetate	13142009	1
	Sodium edetate	20004094011	1
	Sodium edetate	21001224017	1
	Sodium edetate	21122-F04-380679	1
	Sodium edetate	21H12-B03-213591	2
	Sodium edetate	21H12-B03-215577	1
	Sodium edetate	21I22-F04-380679	1
	Sodium edetate	21L06-B01	1
	Sodium edetate	21L06-B01-217364	3
	Sodium edetate	22000319007	7
	Sodium edetate	22000319008	1
	Sodium edetate	22003154003	3
	Sodium edetate	22003154005	1
	Sodium edetate	23A27-B01-230833	1
	Sodium edetate	23A27-B01-235141	1
	Sodium edetate	23A27-B01-235142	1
	Sodium edetate	24C25-B37-001217	1
Alliance Healthcare	Sodium edetate	12181714	1
Alliance Healthcare	Sodium edetate	13E15-N05	2
Alliance Healthcare	Sodium edetate	21001224002	1
Anzag	Sodium edetate	13K19-B02-290051	1
Anzag	Sodium edetate	18H03-B04-358927	1
apoident	Sodium edetate	1807044-01	1
apomix	Sodium edetate	14G03-B05-307737	1
Bombastus	Sodium edetate		1
Bombastus	Sodium edetate	16136404	1
Caelo	Sodium edetate		1
Caelo	Sodium edetate	10887102	1
Caelo	Sodium edetate	11074608	2
Caelo	Sodium edetate	11074703	1
Caelo	Sodium edetate	12181702	1
Caelo	Sodium edetate	12181703	3
Caelo	Sodium edetate	12181704	1
Caelo	Sodium edetate	12181706	2
Caelo	Sodium edetate	12181711	13
Caelo	Sodium edetate	12181714	4
Caelo	Sodium edetate	12254507	2
Caelo	Sodium edetate	12345	1
Caelo	Sodium edetate	12E16-N04	1
Caelo	Sodium edetate	13/23-N03-3472312131	1
Caelo	Sodium edetate	13142002	4
Caelo	Sodium edetate	13142004	4
Caelo	Sodium edetate	13142008	6
Caelo	Sodium edetate	13142009	11
Caelo	Sodium edetate	13142010	2
Caelo	Sodium edetate	13142014	1
Caelo	Sodium edetate	13142015	5
Caelo	Sodium edetate	13142018	2
Caelo	Sodium edetate	13395002	3
Caelo	Sodium edetate	13395007	4
Caelo	Sodium edetate	13E15-N05	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sodium edetate	13E15-N05	1
Caelo	Sodium edetate	13K19-B02-290051	1
Caelo	Sodium edetate	14031801	1
Caelo	Sodium edetate	1427006	1
Caelo	Sodium edetate	14270505	2
Caelo	Sodium edetate	14270506	4
Caelo	Sodium edetate	14G03-B05-307737	1
Caelo	Sodium edetate	15035603	3
Caelo	Sodium edetate	15035604	4
Caelo	Sodium edetate	15116602	4
Caelo	Sodium edetate	15116603	15
Caelo	Sodium edetate	1517E-01925	1
Caelo	Sodium edetate	15427703	15
Caelo	Sodium edetate	15427704	5
Caelo	Sodium edetate	15427705	4
Caelo	Sodium edetate	15427710	13
Caelo	Sodium edetate	15427712	1
Caelo	Sodium edetate	15427714	25
Caelo	Sodium edetate	15427717	11
Caelo	Sodium edetate	1547717	1
Caelo	Sodium edetate	16110103/1	1
Caelo	Sodium edetate	16136403	4
Caelo	Sodium edetate	16136404	5
Caelo	Sodium edetate	16337302	9
Caelo	Sodium edetate	16337305	3
Caelo	Sodium edetate	16337312	24
Caelo	Sodium edetate	16337313	2
Caelo	Sodium edetate	16337316	14
Caelo	Sodium edetate	166337312	1
Caelo	Sodium edetate	16F21-B02-327696	1
Caelo	Sodium edetate	17336102	22
Caelo	Sodium edetate	17336107	5
Caelo	Sodium edetate	17336115	25
Caelo	Sodium edetate	17D25-B08	1
Caelo	Sodium edetate	17d25-b08-339881	1
Caelo	Sodium edetate	17D25-B08-341590	2
Caelo	Sodium edetate	17D25-B08-343253	2
Caelo	Sodium edetate	18007102	13
Caelo	Sodium edetate	18007104	3
Caelo	Sodium edetate	18007110	20
Caelo	Sodium edetate	18007112	3
Caelo	Sodium edetate	18007113	1
Caelo	Sodium edetate	18H03-B03-353918	1
Caelo	Sodium edetate	18H03-B04	1
Caelo	Sodium edetate	18H03-B04-352162	3
Caelo	Sodium edetate	18H03B04356574	1
Caelo	Sodium edetate	18H03-B04-357771	3
Caelo	Sodium edetate	191896007	21
Caelo	Sodium edetate	19189603	7
Caelo	Sodium edetate	200004094004	1
Caelo	Sodium edetate	20004094001	10
Caelo	Sodium edetate	20004094002	1
Caelo	Sodium edetate	20004094004	17
Caelo	Sodium edetate	20004094006	2
Caelo	Sodium edetate	20004094011	4
Caelo	Sodium edetate	20004424015	1
Caelo	Sodium edetate	21001224002	1
Caelo	Sodium edetate	21001224003	14
Caelo	Sodium edetate	21001224005	8
Caelo	Sodium edetate	21001224006	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sodium edetate	21001224013	9
Caelo	Sodium edetate	21001224015	9
Caelo	Sodium edetate	21001224017	5
Caelo	Sodium edetate	21001224019	1
Caelo	Sodium edetate	21001224031	1
Caelo	Sodium edetate	2100128002	1
Caelo	Sodium edetate	2101414	1
Caelo	Sodium edetate	22000319004	2
Caelo	Sodium edetate	22000319007	4
Caelo	Sodium edetate	220304NE	1
Caelo	Sodium edetate	2913M1925	1
Caelo	Sodium edetate	3211I-01925	1
Caelo	Sodium edetate	3913A-01925	1
Caelo	Sodium edetate	601EC350	1
Caelo	Sodium edetate	601EF200	1
Caelo	Sodium edetate	601EH014	1
Caelo	Sodium edetate	92159379	1
Caelo	Sodium edetate	B03-3617200	1
Caelo	Sodium edetate	P-14011921/17336102	1
Caelo	Sodium edetate	P-16061621/15427703	1
Caesar & Loretz GmbH...	Sodium edetate	13142004	1
Caesar & Loretz GmbH...	Sodium edetate	20004094004	1
Caesar & Loretz GmbH Og	Sodium edetate	21001224017	1
Caesar & Loretz GmbH...	Sodium edetate	12181711	1
Caesar & Loretz GmbH...	Sodium edetate	20004094002	1
Caesar & Loretz GmbH...	Sodium edetate	21001224005	1
Caesar & Loretz GmbH/GEHE	Sodium edetate	17336115	1
Caesar & Loretz GmbH/Gehe	Sodium edetate	21001224017	1
Caesar & Loretz GmbH...	Sodium edetate	191896010	1
Caesar & Loretz GmbH...	Sodium edetate	21000128002	1
Caesar & Loretz GmbH...	Sodium edetate	21001224017	1
Caesar & Loretz GmbH/sana	Sodium edetate	21000128002	1
Caesar & Loretz GmbH...	Sodium edetate	16337316	1
Caesar & Loretz GmbH...	Sodium edetate	18007112	1
Caesar & Loretz GmbH...	Sodium edetate	191896007	1
Caesar & Loretz GmbH...	Sodium edetate	21001224005	1
Caesar & Loretz GmbH	Sodium edetate	13142008	1
Caesar & Loretz GmbH	Sodium edetate	14270505	1
Caesar & Loretz GmbH	Sodium edetate	15427705	1
Caesar & Loretz GmbH	Sodium edetate	16337312	1
Caesar & Loretz GmbH	Sodium edetate	17336115	6
Caesar & Loretz GmbH	Sodium edetate	1736115	1
Caesar & Loretz GmbH	Sodium edetate	18007102	1
Caesar & Loretz GmbH	Sodium edetate	18007104	1
Caesar & Loretz GmbH	Sodium edetate	18007110	4
Caesar & Loretz GmbH	Sodium edetate	18007112	1
Caesar & Loretz GmbH	Sodium edetate	18007113	4
Caesar & Loretz GmbH	Sodium edetate	191896007	13
Caesar & Loretz GmbH	Sodium edetate	19189603	3
Caesar & Loretz GmbH	Sodium edetate	20004094001	4
Caesar & Loretz GmbH	Sodium edetate	20004094004	13
Caesar & Loretz GmbH	Sodium edetate	20004094006	3
Caesar & Loretz GmbH	Sodium edetate	20004094011	2
Caesar & Loretz GmbH	Sodium edetate	21001224002	2
Caesar & Loretz GmbH	Sodium edetate	21001224003	1
Caesar & Loretz GmbH	Sodium edetate	21001224005	2
Caesar & Loretz GmbH	Sodium edetate	21001224012	1
Caesar & Loretz GmbH	Sodium edetate	21001224013	3
Caesar & Loretz GmbH	Sodium edetate	21001224015	5
Caesar & Loretz GmbH	Sodium edetate	21001224017	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Sodium edetate	21001224019	1
Caesar & Loretz GmbH	Sodium edetate	22000319004	1
Carl Roth	Sodium edetate	159280302	1
Celo/Noweda	Sodium edetate	18007102	1
Ceolo	Sodium edetate	1909030-01	1
Cranach-Apotheke	Sodium edetate	11a31-no6	1
Delta Apotheke	Sodium edetate	18007102	2
Euro OTC	Sodium edetate	13142018	2
Euro OTC	Sodium edetate	15427703	1
Euro OTC	Sodium edetate	16337312	1
Euro OTC	Sodium edetate	18007110	2
Euro OTC	Sodium edetate	190903001	1
Euro OTC	Sodium edetate	1909030-01	2
Euro OTC	Sodium edetate	2004003-01	1
Euro OTC	Sodium edetate	21001224013	1
Euro OTC	Sodium edetate	E300033328	1
Fagron	Sodium edetate	11A31-N06	1
Fagron	Sodium edetate	11A31-N06Retest	1
Fagron	Sodium edetate	12E12-N04	1
Fagron	Sodium edetate	12E16-N04	2
Fagron	Sodium edetate	12g25-n12	1
Fagron	Sodium edetate	12G25-N12	3
Fagron	Sodium edetate	13/23-N03	6
Fagron	Sodium edetate	13E15-B10-289034	1
Fagron	Sodium edetate	13E15-N05	10
Fagron	Sodium edetate	13G15-N03	4
Fagron	Sodium edetate	13I23-N03	10
Fagron	Sodium edetate	13I23-NO3	1
Fagron	Sodium edetate	13K19B02	1
Fagron	Sodium edetate	13K19-B02	1
Fagron	Sodium edetate	13K19-B02-289035	1
Fagron	Sodium edetate	13k19-b02-290051	2
Fagron	Sodium edetate	13K19B02290051	1
Fagron	Sodium edetate	13K19-B02-290051	11
Fagron	Sodium edetate	13K19-B02-290052	3
Fagron	Sodium edetate	13K19-B02-296324	1
Fagron	Sodium edetate	14G03-B05	5
Fagron	Sodium edetate	14G03-B05_307737	1
Fagron	Sodium edetate	14G03-B05-303420	1
Fagron	Sodium edetate	14G03-B05-303422	1
Fagron	Sodium edetate	14G03-B05-30773	1
Fagron	Sodium edetate	14G03-B05-307737	8
Fagron	Sodium edetate	14G03B05309971	1
Fagron	Sodium edetate	14G03-B05-309971	2
Fagron	Sodium edetate	15D01-B05-315877	4
Fagron	Sodium edetate	15D01-B05-317369	2
Fagron	Sodium edetate	164599-0001	1
Fagron	Sodium edetate	16F21-B02	3
Fagron	Sodium edetate	16F21-B02-323069	1
Fagron	Sodium edetate	16F21-B02-323074	2
Fagron	Sodium edetate	16F21-B02-324370	4
Fagron	Sodium edetate	16f21b02325085	1
Fagron	Sodium edetate	16F21-B02-325085	6
Fagron	Sodium edetate	16F21-B02-325891	3
Fagron	Sodium edetate	16f21-b02-327696	1
Fagron	Sodium edetate	16F21B02327696	1
Fagron	Sodium edetate	16F21-B02-327696	5
Fagron	Sodium edetate	16F21-B02-329900	5
Fagron	Sodium edetate	16f21-b02-330959	1
Fagron	Sodium edetate	16F21-B02-332039	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Sodium edetate	16F21-B02-333607	1
Fagron	Sodium edetate	16F21-B02-333610	3
Fagron	Sodium edetate	17D25-B08	4
Fagron	Sodium edetate	17D25-B08-334827	4
Fagron	Sodium edetate	17D25-B08-334827	1
Fagron	Sodium edetate	17D25-B08-336718	4
Fagron	Sodium edetate	17D25-B08-338202	4
Fagron	Sodium edetate	17D25-B08-339881	4
Fagron	Sodium edetate	17D25B08343253	1
Fagron	Sodium edetate	17D25-B08-343253	4
Fagron	Sodium edetate	17D25-B08-343254	1
Fagron	Sodium edetate	17D25-Bo8-336718	1
Fagron	Sodium edetate	18H03	1
Fagron	Sodium edetate	18H03-B04	3
Fagron	Sodium edetate	18H03-B04-352162	1
Fagron	Sodium edetate	18H03-B04-353034	8
Fagron	Sodium edetate	18H03-B04-353918	6
Fagron	Sodium edetate	18H03-B04-355280	7
Fagron	Sodium edetate	18h03-b04-356574	1
Fagron	Sodium edetate	18H03-B04-356574	6
Fagron	Sodium edetate	18H03-B04-35674	1
Fagron	Sodium edetate	18H03-B04-357771	8
Fagron	Sodium edetate	18H03-B04-357774	8
Fagron	Sodium edetate	18h03b04358927	1
Fagron	Sodium edetate	18H03B04-358927	1
Fagron	Sodium edetate	18H03-B04-358927	6
Fagron	Sodium edetate	18H09-B04-355280	1
Fagron	Sodium edetate	18K14-B03	5
Fagron	Sodium edetate	18K14-B03-358930	13
Fagron	Sodium edetate	18K14-B03-358931	1
Fagron	Sodium edetate	18K14B03358934	1
Fagron	Sodium edetate	18K14-B03-358934	4
Fagron	Sodium edetate	18K14-B03-361720	16
Fagron	Sodium edetate	18K14-B03-361721	1
Fagron	Sodium edetate	20f23	1
Fagron	Sodium edetate	20F23-F03	1
Fagron	Sodium edetate	20F23-F03-372618	6
Fagron	Sodium edetate	21/22-F04	1
Fagron	Sodium edetate	21122-F04_380679	1
Fagron	Sodium edetate	21122-F04-380105	1
Fagron	Sodium edetate	2122-F04-380679	1
Fagron	Sodium edetate	215I-01925	1
Fagron	Sodium edetate	218U-01925	1
Fagron	Sodium edetate	21I22-F04	2
Fagron	Sodium edetate	21I22-F04_380679	1
Fagron	Sodium edetate	21I22-F04-380105	1
Fagron	Sodium edetate	21I22F04380679	1
Fagron	Sodium edetate	21I22-F04-380679	10
Fagron	Sodium edetate	21L06-B01-217364	1
Fagron	Sodium edetate	352162	1
Fagron	Sodium edetate	361720	1
Fagron	Sodium edetate	-37261008	2
Fagron	Sodium edetate	5012Q-01925	1
Fagron	Sodium edetate	5218Q-01925	1
Fagron	Sodium edetate	5315A-01925	1
Fagron	Sodium edetate	601EB174	1
Fagron	Sodium edetate	601EB262	1
Fagron	Sodium edetate	601EC350	2
Fagron	Sodium edetate	601EE047	3
Fagron	Sodium edetate	601EF172	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Sodium edetate	601EF200	5
Fagron	Sodium edetate	601EH014	1
Fagron	Sodium edetate	601EI153	2
Fagron	Sodium edetate	601H1300	2
Fagron	Sodium edetate	601H9118	1
Fagron	Sodium edetate	601HA062	6
Fagron	Sodium edetate	6O1EI153	1
Fagron	Sodium edetate	813Q-01925	1
Fagron	Sodium edetate	914E-01925	1
Fagron	Sodium edetate	B01-2173006	1
Fagron	Sodium edetate	B03-2135901	1
Fagron	Sodium edetate	B03-3617200	1
Fagron	Sodium edetate	B03-3617201	1
Fagron	Sodium edetate	F03-3726108	2
Fagron	Sodium edetate	FO4-3806709	1
Fagron	Sodium edetate	NE5736385	1
Fargo/Phönix	Sodium edetate	18K14-B03	1
Fargo/Sana	Sodium edetate	20004094006	1
Fargon/Noweda	Sodium edetate	18H03-B04-356574	2
Fargon/Phönix	Sodium edetate	BO3-3617201	1
Fargon	Sodium edetate	18H03-B04	1
Fargon	Sodium edetate	18H03-B04-353034	1
Fargron / Noweda	Sodium edetate	16f21-b0-330959	1
Fiebig	Sodium edetate	16F21-B02-327696	1
Fiebig	Sodium edetate	18007110	1
Fragon/Noweda	Sodium edetate	18H03-B04-358927	1
Gehe	Sodium edetate	13142018	1
Gehe	Sodium edetate	13E15-N05	1
Gehe	Sodium edetate	15427710	1
Gehe	Sodium edetate	21L06-B01-217364	1
Gehe	Sodium edetate	22003154005	1
Kehr/Fargon	Sodium edetate	17d25-b08-343253	1
kehr	Sodium edetate	17D25-B08-339881	1
Kehr	Sodium edetate	21L06-B01	1
Noweda/Gehe	Sodium edetate	14G03-B05-307737	1
Noweda	Sodium edetate	15427710	1
Noweda	Sodium edetate	16337312	1
Noweda	Sodium edetate	18K14-B03-361720	1
Noweda	Sodium edetate	601H1300	1
Noweda	Sodium edetate	B03-3617200	1
Phoenix Goettin	Sodium edetate	13G15-N03	1
Phoenix Goettin	Sodium edetate	13G15-NO3	1
Phoenix	Sodium edetate	15427704	1
Phoenix	Sodium edetate	16F21-B02-333607	1
Phoenix	Sodium edetate	18007110	1
Phoenix	Sodium edetate	3411	1
Phönix	Sodium edetate	11074702	1
Phönix	Sodium edetate	13142004	1
phönix	Sodium edetate	13142018	1
Phönix	Sodium edetate	13E15-B10	1
Phönix	Sodium edetate	13G15-N03	1
phönix	Sodium edetate	13K19-B02-290051	1
phönix	Sodium edetate	15427703	1
phönix	Sodium edetate	15427704	1
Phönix	Sodium edetate	164599-0001	1
Phönix	Sodium edetate	16F21-B02-327696	1
Phönix	Sodium edetate	18007110	1
Phönix	Sodium edetate	18H03-B04-353034	1
Phönix	Sodium edetate	18K14-B03-358930	2
Phönix	Sodium edetate	200471805	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Sodium edetate	601ef200	1
Röntgen	Sodium edetate	16337302	1
Röntgen	Sodium edetate	20004094001	1
Sanacorp	Sodium edetate	12G25-N12	2
Sanacorp	Sodium edetate	13E15-N05	1
Sanacorp	Sodium edetate	1505603	1
Sanacorp	Sodium edetate	164599-0001	1
sanacorp	Sodium edetate	16F21-B02-324370	1
Sanacorp	Sodium edetate	17336115	1
Sanacorp	Sodium edetate	20004094004	1
Sanacorp	Sodium edetate	21h12-b03-213591	2
Sanacorp	Sodium edetate	21i22-F04-380679	1
Sanacorp	Sodium edetate	21L06-B01-217364	2
Sanacorp	Sodium edetate	22000319007	1
Sanacorp	Sodium edetate	6/AKD14	1
VDL	Sodium edetate	22000319008	1
Vincenten/ Sanacorp	Sodium edetate	18K14-B03-3617200	1

- 235 023 spectra from 1515 *Apo-Ident* customers from a total of 49 012 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sodium edetate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sodium edetate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	760	0	201 324
Type C	0	1042	2	235 023

The substance/substance group *Sodium edetate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2105 %)
Type C	100.0000 % (> 99.9007 %)	99.8084 % (> 99.5211 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20937	20937	0.00	143.08
21362	22465	5.26	142.91
22465	22465	0.00	145.01
22915	22915	0.00	144.31
22926	22465	8.03	142.38
24414	24414	0.00	141.81
26394	20937	7.34	144.99

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sodium salicylate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21037-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium salicylate; Natrii salicylas

Special notes

When selecting the *Sodium salicylate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sodium salicylate	4	3	7

Second-stage model

For differentiation of the substance/substance group *Sodium salicylate* the following second-stage model is used:

- Submodel 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sodium salicylate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Dithranol	74.88	16.20
⋮	⋮	⋮
Dequalinium chloride	>50	50.47
Benzoic acid	>50	51.09
Acetylsalicylic acid	>50	104.30
Eosin Y	>50	156.74
Oxytetracycline hydrochloride	>50	261.41
Levothyroxin sodium	>50	580.74
Tannin	>50	1207.07

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sodium salicylate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sodium salicylate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium salicylate	12158307	21037	40	1403225
Caelo	Sodium salicylate	13140513	21689	60	20130531
Caelo	Sodium salicylate	163053	23052	40	20161118*
Gatt-Koller	Sodium salicylate	22J02278	26705	40	20221206

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 180 spectra of 4 reference samples from the substance/substance group *Sodium salicylate*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 152 782 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 5 reference samples from the substance/substance group *Sodium salicylate*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium salicylate	16305301	22879	40
Caelo	Sodium salicylate	20002958001	25428	40
Gatt-Koller	Sodium salicylate	23J02384	27094	40
Gatt-Koller	Sodium salicylate	22J02278	26705SI†	20
Gatt-Koller	Sodium salicylate	23J02384	27094SI	20

- 201 924 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 8 spectra from 6 *Apo-Ident* customers from 7 batches from the substance/substance group *Sodium salicylate*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Sodium salicylate	18061305	1
Caelo	Sodium salicylate	20002958001	1
Caesar & Loretz GmbH…	Sodium salicylate	20004439001	2
Fagron	Sodium salicylate	102091210	1
GATT-KOLLER/PHOENIX	Sodium salicylate	4853/11124512	1
Gehe	Sodium salicylate	13G31-B03-287961	1
Phoenix	Sodium salicylate	12158309	1

- 236 059 spectra from 1515 *Apo-Ident* customers from a total of 49 251 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sodium salicylate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sodium salicylate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	180	0	152 782
Type B	0	160	0	201 924
Type C	0	8	0	236 059

The substance/substance group *Sodium salicylate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.6667 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21037	21037	0.00	197.10
21689	21037	5.69	197.05
23052	23052	0.00	185.91
26705	21037	26.70	181.82

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sodium sulfate decahydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20124-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium sulfate decahydrate; Natrii sulfas decahydricus; Sodium sulphate decahydrate

Special notes

When selecting the *Sodium sulfate decahydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sodium sulfate decahydrate	2	2	29

Second-stage model

For differentiation of the substance/substance group *Sodium sulfate decahydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sodium sulfate decahydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	81.39	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sodium sulfate decahydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sodium sulfate decahydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium sulfate decahydrate	23001158	27082	40	20230609*
Caelo	Sodium sulfate decahydrate	23001158	27082SI	20	20230609*
Euro OTC	Sodium sulfate decahydrate	2111018	26149	40	20211126*
Euro OTC	Sodium sulfate decahydrate	2111018	26149SI	20	20211126*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 120 spectra of 4 reference samples from the substance/substance group *Sodium sulfate decahydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 842 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 100 spectra of 3 reference samples from the substance/substance group *Sodium sulfate decahydrate*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Sodium sulfate decahydrate	1708012-02	24274	40
Euro OTC	Sodium sulfate decahydrate	2301001	27086	40
Euro OTC	Sodium sulfate decahydrate	2301001	27086SI	20

- 201 984 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 73 spectra from 29 *Apo-Ident* customers from 29 batches from the substance/substance group *Sodium sulfate decahydrate*.

- Among them are spectra of independent samples from 29 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caaelo	Sodium sulfate decahydrate	11294603	2
Caelo	Sodium sulfate decahydrate	11012207	1
Caelo	Sodium sulfate decahydrate	11012210	2
Caelo	Sodium sulfate decahydrate	12157001	1
Caelo	Sodium sulfate decahydrate	12157005	13
Caelo	Sodium sulfate decahydrate	12157006	3
Caelo	Sodium sulfate decahydrate	12157007	1
Caelo	Sodium sulfate decahydrate	12157011	1
Caelo	Sodium sulfate decahydrate	12157012	18

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sodium sulfate decahydrate	12157013	1
Caelo	Sodium sulfate decahydrate	12256902	1
Caelo	Sodium sulfate decahydrate	12257901	1
Caelo	Sodium sulfate decahydrate	12257902	5
Caelo	Sodium sulfate decahydrate	18101202	1
Caelo	Sodium sulfate decahydrate	205026	1
Caelo	Sodium sulfate decahydrate	61599506	1
Caelo	Sodium sulfate decahydrate	70706387	1
EuRho	Sodium sulfate decahydrate	1210005-01	1
Euro OTC	Sodium sulfate decahydrate	1108035-01	3
Euro OTC	Sodium sulfate decahydrate	1108035-02	2
Euro OTC	Sodium sulfate decahydrate	121000502	2
Euro OTC	Sodium sulfate decahydrate	1210005-02	2
Euro OTC	Sodium sulfate decahydrate	4312I-01920	1
Fagron	Sodium sulfate decahydrate	1464	1
Fagron	Sodium sulfate decahydrate	2134	1
fargon/Sanacorp	Sodium sulfate decahydrate	12H31-N04	1
Fiebig 29.04.13 ek: 5,64EUR	Sodium sulfate decahydrate	1210005-01	1
Gehe	Sodium sulfate decahydrate	12257902	1
Hedinger/Phönix	Sodium sulfate decahydrate	205025	1
nachprüfung	Sodium sulfate decahydrate	C1069	1
Unisan	Sodium sulfate decahydrate	11294605	1

- 235 994 spectra from 1515 *Apo-Ident* customers from a total of 49 229 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sodium sulfate decahydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sodium sulfate decahydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	120	0	152 842
Type B	0	100	0	201 984
Type C	0	73	0	235 994

The substance/substance group *Sodium sulfate decahydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 94.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 91.7808 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26149	26149	0.00	156.16
27082	27082	0.00	166.48

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sodium tetraborate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20179-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sodium tetraborate; Borax

Special notes

When selecting the *Sodium tetraborate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sodium tetraborate	9	13	33

Second-stage model

For differentiation of the substance/substance group *Sodium tetraborate* the following second-stage model is used:

- Submodel 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sodium tetraborate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	48.14	–
Sodium dihydrogen phosphate dihydrate	76.04	–
⋮	⋮	⋮
Magnesium citrate	>50	56.34
Riboflavin sodium phosphate hydrate	>50	59.83
Carbomers	>50	121.43
Gentamicin sulfate	>50	128.64
Mg-Ca-K colamine phosphate	>50	184.11
Zinc gluconate	>50	195.85
Tobramycin sulfate	>50	256.23
Neomycin sulfate	>50	273.82
Finasteride	>50	1638.12

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sodium tetraborate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sodium tetraborate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sodium tetraborate	13290118	21438	60	1412042
Caelo	Sodium tetraborate	161372	22475	60	20160624*
Caelo	Sodium tetraborate	161372	22621	40	20160624*
Euro OTC	Sodium tetraborate	1404025-01	21656	60	20140514
Euro OTC	Sodium tetraborate	1507024	21854	60	20150730*
Euro OTC	Sodium tetraborate	1510032	22235	60	20151118*
Euro OTC	Sodium tetraborate	1711002	23892	40	20171128*
Euro OTC	Sodium tetraborate	2004009	25150	40	20200511*
Euro OTC	Sodium tetraborate	2008006	25350	40	20200904*
Euro OTC	Sodium tetraborate	2107002	25770	40	20210727*
Euro OTC	Sodium tetraborate	2107002	25770SI	40	20210727*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 540 spectra of 11 reference samples from the substance/substance group *Sodium tetraborate*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.
- 152 422 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 940 spectra of 23 reference samples from the substance/substance group *Sodium tetraborate*.
- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sodium tetraborate	21000651002	25985	40
Caelo	Sodium tetraborate	24000302	27244	40
Euro OTC	Sodium tetraborate	1603043	22508	40
Euro OTC	Sodium tetraborate	1607036	22713	40
Euro OTC	Sodium tetraborate	1701046	22990	40
Euro OTC	Sodium tetraborate	1804014	24093	40
Euro OTC	Sodium tetraborate	2111003	25895	50
Euro OTC	Sodium tetraborate	2202006	25944	40
Euro OTC	Sodium tetraborate	2202007	25956	40
Euro OTC	Sodium tetraborate	2202005	25968	40
Euro OTC	Sodium tetraborate	2209019	26334	40
Euro OTC	Sodium tetraborate	2307005	26885	40
Euro OTC	Sodium tetraborate	2310017	27000	40
Caelo	Sodium tetraborate	21000651002	25985SI	40
Caelo	Sodium tetraborate	24000302	27244SI	40
Euro OTC	Sodium tetraborate	2008006	25350SI†	40
Euro OTC	Sodium tetraborate	2111003	25895SI	50

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Sodium tetraborate	2202006	25944SI	40
Euro OTC	Sodium tetraborate	2202007	25956SI	40
Euro OTC	Sodium tetraborate	2202005	25968SI	40
Euro OTC	Sodium tetraborate	2209019	26334SI	40
Euro OTC	Sodium tetraborate	2307005	26885SI	40
Euro OTC	Sodium tetraborate	2310017	27000SI	40

- 201 144 spectra from a total of 4031 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 57 spectra from 44 *Apo-Ident* customers from 35 batches from the substance/substance group *Sodium tetraborate*.

- Among them are spectra of independent samples from 33 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sodium tetraborate	2202006-01	1
	Sodium tetraborate	2310017-01	1
	Sodium tetraborate	2310017-02	2
Borax Francais	Sodium tetraborate	1402002-01	1
Caelo	Sodium tetraborate	11369412	1
Caelo	Sodium tetraborate	11369431	1
Caelo	Sodium tetraborate	1309032-01	1
Caelo	Sodium tetraborate	13290118	1
Caelo	Sodium tetraborate	14310905	2
Caelo	Sodium tetraborate	150702401	1
Caelo	Sodium tetraborate	1607036-01	1
Caelo	Sodium tetraborate	16081801	1
Caelo	Sodium tetraborate	16137201	1
Caelo	Sodium tetraborate	16137205	1
Caelo	Sodium tetraborate	21051402	1
Caesar & Loretz GmbH	Sodium tetraborate	20000902001	1
EuRho	Sodium tetraborate	1607036-01	2
Euro OTC	Sodium tetraborate		1
Euro OTC	Sodium tetraborate	130203401	1
Euro OTC	Sodium tetraborate	1302034-01	1
Euro OTC	Sodium tetraborate	1309032-01	1
Euro OTC	Sodium tetraborate	13111207	1
Euro OTC	Sodium tetraborate	1408006-01	1
Euro OTC	Sodium tetraborate	1503043-01	1
Euro OTC	Sodium tetraborate	1507024-01	3
Euro OTC	Sodium tetraborate	160304301	1
Euro OTC	Sodium tetraborate	1607036-01	2
Euro OTC	Sodium tetraborate	1701046-01	1
Euro OTC	Sodium tetraborate	1711002-01	8

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Sodium tetraborate	1804014-01	3
Euro OTC	Sodium tetraborate	2004009-01	1
Euro OTC	Sodium tetraborate	2008006-01	3
Euro OTC	Sodium tetraborate	2107002-01	2
Euro OTC	Sodium tetraborate	22020005-01	1
Euro/Alliance Healthcare	Sodium tetraborate	171100201	1
Fagron	Sodium tetraborate	12H09-N03	1
Gatt-Koller / Phoenix	Sodium tetraborate	6187/01142114	1
Phoenix	Sodium tetraborate	1603043-01	1
Sanacorp	Sodium tetraborate	171100201	1

- 236 010 spectra from 1515 *Apo-Ident* customers from a total of 49 224 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sodium tetraborate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sodium tetraborate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	540	0	152 422
Type B	0	940	0	201 144
Type C	0	57	0	236 010

The substance/substance group *Sodium tetraborate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8889 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.3617 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 89.4737 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21438	21438	0.00	127.66
21656	22475	8.29	129.24
21854	21854	0.00	112.54
22235	22235	0.00	114.20
22475	22475	0.00	124.98
22621	22621	0.00	122.44
23892	23892	0.00	101.40
25150	25150	0.00	127.34
25350	25350	0.00	101.59
25770	25770	0.00	127.29

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sorbic acid**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20881-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sorbic acid; Acidum sorbicum

Special notes

When selecting the *Sorbic acid* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sorbic acid	9	3	110

Second-stage model

For differentiation of the substance/substance group *Sorbic acid* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sorbic acid* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	81.33	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sorbic acid* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sorbic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sorbic acid	12038025	20881	40	20120315
Caelo	Sorbic acid	13334008	21460	60	AR-15-FG-007849-01
Caelo	Sorbic acid	14380714	22593	40	20150209
Caelo	Sorbic acid	162080	22616	40	20160722*
Caelo	Sorbic acid	15382002	22826	40	20151112
Caelo	Sorbic acid	172056	23851	40	20170823*
Caelo	Sorbic acid	162080	23859	40	20160722*
Caelo	Sorbic acid	20002774	25615	40	20200910*
Caelo	Sorbic acid	22000825	26120	40	20220513*
Caelo	Sorbic acid	22000825	26120SI	20	20220513*
Caelo	Sorbic acid	23002243	26951	40	20230914*
Caelo	Sorbic acid	23002243	26951SI	20	20230914*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 460 spectra of 12 reference samples from the substance/substance group *Sorbic acid*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 502 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Sorbic acid*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sorbic acid	14176214	22592	40
Caelo	Sorbic acid	182876	24384	40
Caelo	Sorbic acid	191114	24569	40

- 201 964 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 772 spectra from 459 *Apo-Ident* customers from 117 batches from the substance/substance group *Sorbic acid*.

- Among them are spectra of independent samples from 110 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sorbic acid	22000825005	1
	Sorbic acid	22000825006	1
	Sorbic acid	22000825009	1
	Sorbic acid	22000825011	1
	Sorbic acid	22000825015	1
	Sorbic acid	22000825016	3
	Sorbic acid	22000825020	4
	Sorbic acid	22000825105	1
	Sorbic acid	22000825106	1
	Sorbic acid	23002243003	2
acidum sorbicum	Sorbic acid	17343411	1
AHD	Sorbic acid	22000825020	1
ALH	Sorbic acid	15382007	1
Alliance Healthcare	Sorbic acid	20000110010	1
Alliance Healthcare	Sorbic acid	20004209014	1
Alliance	Sorbic acid	22000825020	1
Anzag	Sorbic acid	12038016	1
Caelo	Sorbic acid		1
Caelo	Sorbic acid	10120303	1
Caelo	Sorbic acid	10305208	1
Caelo	Sorbic acid	10305209	1
Caelo	Sorbic acid	105505	1
Caelo	Sorbic acid	11203806	2
Caelo	Sorbic acid	11203807	10
Caelo	Sorbic acid	11203812	1
Caelo	Sorbic acid	12038002	1
Caelo	Sorbic acid	12038009	1
Caelo	Sorbic acid	12038012	1
Caelo	Sorbic acid	12038016	6
Caelo	Sorbic acid	12038020	4
Caelo	Sorbic acid	12038025	1
Caelo	Sorbic acid	12330608	8
Caelo	Sorbic acid	12330618	12
Caelo	Sorbic acid	13334003	4
Caelo	Sorbic acid	13334008	6
Caelo	Sorbic acid	13334010	7
Caelo	Sorbic acid	14176206	7
Caelo	Sorbic acid	14176207	1
Caelo	Sorbic acid	14176209	6
Caelo	Sorbic acid	14176212	8
Caelo	Sorbic acid	14176213	1
Caelo	Sorbic acid	14176214	12
Caelo	Sorbic acid	14380702	3
Caelo	Sorbic acid	14380704	1
Caelo	Sorbic acid	14380706	6
Caelo	Sorbic acid	14380713	2
Caelo	Sorbic acid	14380714	11
Caelo	Sorbic acid	14380715	1
Caelo	Sorbic acid	15123912	1
Caelo	Sorbic acid	15382001	1
Caelo	Sorbic acid	15382002	12
Caelo	Sorbic acid	15382007	4
Caelo	Sorbic acid	15382010	15
Caelo	Sorbic acid	16206012	1
Caelo	Sorbic acid	162080	1
Caelo	Sorbic acid	16208005	30
Caelo	Sorbic acid	16208007	1
Caelo	Sorbic acid	16208009	22
Caelo	Sorbic acid	16208011	13
Caelo	Sorbic acid	16208012	8

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sorbic acid	16208015	12
Caelo	Sorbic acid	16208016	18
Caelo	Sorbic acid	16208018	2
Caelo	Sorbic acid	16208020	18
Caelo	Sorbic acid	1620808005	1
Caelo	Sorbic acid	162508016	1
Caelo	Sorbic acid	170427AS/16208005	1
Caelo	Sorbic acid	1734301	1
Caelo	Sorbic acid	17343401	17
Caelo	Sorbic acid	17343411	26
Caelo	Sorbic acid	17343411P-190225-13	1
Caelo	Sorbic acid	17343422	16
Caelo	Sorbic acid	18215610	1
Caelo	Sorbic acid	1827669	1
Caelo	Sorbic acid	18284605	1
Caelo	Sorbic acid	18286716	1
Caelo	Sorbic acid	18287602	2
Caelo	Sorbic acid	18287605	30
Caelo	Sorbic acid	18287609	27
Caelo	Sorbic acid	18287616	22
Caelo	Sorbic acid	18287616P-191111-5	1
Caelo	Sorbic acid	1887618	1
Caelo	Sorbic acid	191114	1
Caelo	Sorbic acid	191114001	20
Caelo	Sorbic acid	191114002	22
Caelo	Sorbic acid	19111405	1
Caelo	Sorbic acid	19114002	2
Caelo	Sorbic acid	200000110010	1
Caelo	Sorbic acid	20000110010	6
Caelo	Sorbic acid	200004209003	2
Caelo	Sorbic acid	20004209003	24
Caelo	Sorbic acid	20004209011	15
Caelo	Sorbic acid	20004209014	17
Caelo	Sorbic acid	2000420911	1
Caelo	Sorbic acid	200042209011	1
Caelo	Sorbic acid	21041801	1
Caelo	Sorbic acid	22000825005	4
Caelo	Sorbic acid	22000825006	4
Caelo	Sorbic acid	22000825009	2
Caelo	Sorbic acid	22000825015	1
Caelo	Sorbic acid	22000825016	5
Caelo	Sorbic acid	22000825020	1
Caelo	Sorbic acid	28041726	1
Caelo	Sorbic acid	29071201	1
Caelo	Sorbic acid	4016I-01048	1
Caelo	Sorbic acid	4811Q-01048	1
Caelo	Sorbic acid	5012E-01048	1
Caelo	Sorbic acid	72687038	1
Caelo	Sorbic acid	80538258	1
Caelo	Sorbic acid	9280207	1
Caelo	Sorbic acid	93557220	2
Caelo	Sorbic acid	P0538258	1
Caeo/ Phoenix	Sorbic acid	18287616	1
Caesar & Lorenz GmbH	Sorbic acid	18287609	1
Caesar & Loretz GmbH...	Sorbic acid	191114001	1
Caesar & Loretz GmbH...	Sorbic acid	18287616	1
Caesar & Loretz GmbH...	Sorbic acid	16208009	1
Caesar & Loretz GmbH...	Sorbic acid	191114002	1
Caesar & Loretz GmbH...	Sorbic acid	18287616	1
Caesar & Loretz GmbH...	Sorbic acid	19111405	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Sorbic acid	22000825006	1
Caesar & Loretz GmbH...	Sorbic acid	20000110005	1
Caesar & Loretz GmbH...	Sorbic acid	19111406	1
Caesar & Loretz GmbH/Gehe	Sorbic acid	191114001	1
Caesar & Loretz GmbH/Gehe	Sorbic acid	191114002	1
Caesar & Loretz GmbH/Gehe	Sorbic acid	22000825006	2
Caesar & Loretz GmbH...	Sorbic acid	18287609	1
Caesar & Loretz GmbH...	Sorbic acid	191114001	1
Caesar & Loretz GmbH...	Sorbic acid	20004209003	1
Caesar & Loretz GmbH/K	Sorbic acid	20004209014	1
Caesar & Loretz GmbH...	Sorbic acid	191114001	1
Caesar & Loretz GmbH...	Sorbic acid	20000110005	1
Caesar & Loretz GmbH...	Sorbic acid	20000110010	1
Caesar & Loretz GmbH...	Sorbic acid	20004209003	1
Caesar & Loretz GmbH/Sana	Sorbic acid	18287606	1
Caesar & Loretz GmbH...	Sorbic acid	191114005	1
Caesar & Loretz GmbH...	Sorbic acid	20000110010	1
Caesar & Loretz GmbH...	Sorbic acid	20004209003	1
Caesar & Loretz GmbH...	Sorbic acid	20004209006	1
Caesar & Loretz GmbH...	Sorbic acid	20004209011	1
Caesar & Loretz GmbH...	Sorbic acid	22000825016	1
Caesar & Loretz GmbH	Sorbic acid	18287605	7
Caesar & Loretz GmbH	Sorbic acid	18287609	7
Caesar & Loretz GmbH	Sorbic acid	18287615	1
Caesar & Loretz GmbH	Sorbic acid	18287616	12
Caesar & Loretz GmbH	Sorbic acid	191114001	11
Caesar & Loretz GmbH	Sorbic acid	191114002	2
Caesar & Loretz GmbH	Sorbic acid	20000110010	2
Caesar & Loretz GmbH	Sorbic acid	20004209002	1
Caesar & Loretz GmbH	Sorbic acid	20004209003	7
Caesar & Loretz GmbH	Sorbic acid	20004209008	1
Caesar & Loretz GmbH	Sorbic acid	20004209010	4
Caesar & Loretz GmbH	Sorbic acid	20004209011	2
Caesar & Loretz GmbH	Sorbic acid	20004209014	9
Caesar & Loretz GmbH	Sorbic acid	22000825006	1
Caesar & Loretz GmbH	Sorbic acid	22000825009	1
Caesar & Loretz GmbH	Sorbic acid	22000825020	1
Caesar & Loretz GmbH	Sorbic acid	22000825105	1
Caesar & Loretz GmbH	Sorbic acid	22000825106	1
Caesar & Loretz/Noweda	Sorbic acid	14380706	1
Caesar/Gehe	Sorbic acid	17343422	1
Cealo/Gehe	Sorbic acid	22000825009	1
Cealo	Sorbic acid	16208011	1
Ebert & Jacobi	Sorbic acid	16208005	1
Euro OTC	Sorbic acid	12038020	1
Euro OTC	Sorbic acid	o216E-01048	1
Fagron	Sorbic acid	121394	1
Fagron	Sorbic acid	13334008	1
Fagron	Sorbic acid	14176206	1
Fagron	Sorbic acid	17343422	1
Fiebig	Sorbic acid	168009	1
Finze	Sorbic acid	9280207	1
Fischar	Sorbic acid	16208005	1
Gatt-Koller / Phoenix	Sorbic acid	2575/07142914	1
Gehe Rostock	Sorbic acid	191114001	1
Gehe	Sorbic acid	16208011	1
Gehe	Sorbic acid	16208012	1
gehe	Sorbic acid	16208016	1
Gehe	Sorbic acid	17343401	1
GEHE	Sorbic acid	17343401	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Sorbic acid	18287605	1
Gehe	Sorbic acid	18287609	2
Gehe	Sorbic acid	191114002	1
Gehe	Sorbic acid	20004209011	1
Geilenkirchen	Sorbic acid	16208009	1
H.Lamotte	Sorbic acid	17343401	1
L12	Sorbic acid	15382010	1
L12	Sorbic acid	18287602	1
Noweda	Sorbic acid	12038016	1
Noweda	Sorbic acid	12330608	1
Noweda	Sorbic acid	14176206	1
Noweda	Sorbic acid	1418M-01048	1
Noweda	Sorbic acid	14380706	1
Noweda	Sorbic acid	16208020	1
Noweda	Sorbic acid	18287605	3
Noweda	Sorbic acid	18287609	1
Noweda	Sorbic acid	20000110010	1
Noweda	Sorbic acid	22000825011	1
Noweda	Sorbic acid	22000825020	1
Phoenix 17.4.13	Sorbic acid	12038020	1
PHOENIX 12.05.2014	Sorbic acid	13334008	1
Phoenix 22.03.2017 6,67EUR	Sorbic acid	15382010	1
Phoenix	Sorbic acid	11203813	1
Phoenix	Sorbic acid	191114001	1
Phoenix	Sorbic acid	20004209003	1
Phönix	Sorbic acid	12330618	1
phönix	Sorbic acid	15382010	1
Phönix	Sorbic acid	16208005	1
Phönix	Sorbic acid	16208020	1
Phönix	Sorbic acid	18287605	1
Phönix	Sorbic acid	20000110010	1
PHÖNIX	Sorbic acid	9308627	1
Sanacorp	Sorbic acid	12038016	1
Sanacorp	Sorbic acid	13334008	1
Sanacorp	Sorbic acid	16208020	1
Sanacorp	Sorbic acid	18287605	2
Sanacorp	Sorbic acid	20004209003	1
Sanacorp	Sorbic acid	22000825006	1
Sanacorp	Sorbic acid	22000825008	1
SanacorpWE: 23.09.14...	Sorbic acid	14176212	1
Th. Geyer	Sorbic acid	17343411	1
vdl 28.04.2014 preis:5,79	Sorbic acid		1
VDL;5,78EUR;18.12	Sorbic acid	14176206	1

- 235 295 spectra from 1515 *Apo-Ident* customers from a total of 49 143 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sorbic acid* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sorbic acid* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	460	0	152 502
Type B	0	120	0	201 964
Type C	0	772	0	235 295

The substance/substance group *Sorbic acid* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6957 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 99.2228 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20881	23859	7.07	140.34
21460	21460	0.00	140.45
22593	23859	5.59	141.38
22616	22616	0.00	145.13
22826	21460	8.19	137.43
23851	23851	0.00	139.52
23859	23859	0.00	139.82
25615	25615	0.00	137.01
26120	26120	0.00	151.97
26951	26951	0.00	159.36

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sorbitol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20075-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sorbitol; Sorbitolum

Special notes

When selecting the *Sorbitol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sorbitol	9	14	151

Second-stage model

For differentiation of the substance/substance group *Sorbitol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sorbitol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Xylitol	68.08	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sorbitol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sorbitol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sorbitol	13278217	21485	40	20130920
Caelo	Sorbitol	16038501	22847	40	20160315
Caelo	Sorbitol	163531	23028	40	20170119*
Caelo	Sorbitol	16353107	23442	40	20170119
Caelo	Sorbitol	20001873	25226	40	20200722*
Euro OTC	Sorbitol	1506052	21834	60	20150713*
Euro OTC	Sorbitol	1512016	22293	60	20160113*
Euro OTC	Sorbitol	1604007	22539	40	20160428*
Euro OTC	Sorbitol	1610018	22849	40	20161121*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 400 spectra of 9 reference samples from the substance/substance group *Sorbitol*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 562 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 680 spectra of 20 reference samples from the substance/substance group *Sorbitol*.

- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sorbitol	181636	24220	40
Caelo	Sorbitol	190173	24562	40
Caelo	Sorbitol	192579	24898	40
Caelo	Sorbitol	22003595	26503	40
Caelo	Sorbitol	23000792	26707	40
Caelo	Sorbitol	24000391	27252	40
Euro OTC	Sorbitol	1810010	24306	40
Euro OTC	Sorbitol	2008016	25333	40
Euro OTC	Sorbitol	2108021	25878	50
Euro OTC	Sorbitol	2207023	26271	40
Euro OTC	Sorbitol	2407005	27396	40
Euro OTC	Sorbitol	2411016	27463	40
Fagron	Sorbitol	22B07-B02-218419	26153	40
Fagron	Sorbitol	22J22-B02	26446	40
Caelo	Sorbitol	22003595	26503SI	20
Euro OTC	Sorbitol	2108021	25878SI	10
Euro OTC	Sorbitol	2207023	26271SI	20
Euro OTC	Sorbitol	2407005	27396SI	20
Euro OTC	Sorbitol	2411016	27463SI	20
Fagron	Sorbitol	22B07-B02-218419	26153SI	20

- 201 404 spectra from a total of 4031 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 459 spectra from 187 *Apo-Ident* customers from 156 batches from the substance/substance group *Sorbitol*.
- Among them are spectra of independent samples from 150 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sorbitol	21003580009	1
	Sorbitol	2108021-01	1
	Sorbitol	22003595002	1
	Sorbitol	22003595005	4
	Sorbitol	22003595007	1
	Sorbitol	22003595008	2
	Sorbitol	22003595009	1
	Sorbitol	23000792004	1
Bombastus	Sorbitol	13278206	2
Caela/ L2	Sorbitol	16038501	1
Caelo	Sorbitol		1
Caelo	Sorbitol	10383323	1
Caelo	Sorbitol	1083330	1
Caelo	Sorbitol	113793	1
Caelo	Sorbitol	11379320	1
Caelo	Sorbitol	11379321	1
Caelo	Sorbitol	11379322	1
Caelo	Sorbitol	11379332	2
Caelo	Sorbitol	11379333	1
Caelo	Sorbitol	11379336	2
Caelo	Sorbitol	11379337	2
Caelo	Sorbitol	12249108	2
Caelo	Sorbitol	12249109	2
Caelo	Sorbitol	12249110	4
Caelo	Sorbitol	12249124	2
Caelo	Sorbitol	12249126	2
Caelo	Sorbitol	12249139	1
Caelo	Sorbitol	12249140	1
Caelo	Sorbitol	12345	1
Caelo	Sorbitol	12L07-N12	1
Caelo	Sorbitol	13278204	1
Caelo	Sorbitol	13278206	1
Caelo	Sorbitol	13278216	2
Caelo	Sorbitol	13278218	1
Caelo	Sorbitol	13278239	1
Caelo	Sorbitol	13278241	1
Caelo	Sorbitol	13278246	2
Caelo	Sorbitol	13278247	1
Caelo	Sorbitol	13278249	1
Caelo	Sorbitol	13278250	1
Caelo	Sorbitol	133335307	1
Caelo	Sorbitol	13335304	1
Caelo	Sorbitol	13335307	3
Caelo	Sorbitol	14250806	1
Caelo	Sorbitol	14250807	1
Caelo	Sorbitol	14250808	1
Caelo	Sorbitol	15012708	1
Caelo	Sorbitol	15118901	3
Caelo	Sorbitol	15118902	2
Caelo	Sorbitol	15118912	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sorbitol	1512016-01	2
Caelo	Sorbitol	15208302	4
Caelo	Sorbitol	15208303	1
Caelo	Sorbitol	15208305	4
Caelo	Sorbitol	15208306	4
Caelo	Sorbitol	15208309	3
Caelo	Sorbitol	15208310	5
Caelo	Sorbitol	15208311	3
Caelo	Sorbitol	16038501	5
Caelo	Sorbitol	16038502	3
Caelo	Sorbitol	16038503	1
Caelo	Sorbitol	16038514	9
Caelo	Sorbitol	16038515	9
Caelo	Sorbitol	1604007-01	1
Caelo	Sorbitol	1610018-01	1
Caelo	Sorbitol	16101303	1
Caelo	Sorbitol	16231208	1
Caelo	Sorbitol	162353107	1
Caelo	Sorbitol	16353102	3
Caelo	Sorbitol	16353107	2
Caelo	Sorbitol	16353108	6
Caelo	Sorbitol	17011305	1
Caelo	Sorbitol	17140902	9
Caelo	Sorbitol	17140903	14
Caelo	Sorbitol	17140904	2
Caelo	Sorbitol	1714090903	1
Caelo	Sorbitol	17366301	15
Caelo	Sorbitol	17366304	9
Caelo	Sorbitol	17366305	2
Caelo	Sorbitol	18163605	2
Caelo	Sorbitol	18163606	9
Caelo	Sorbitol	18163607	9
Caelo	Sorbitol	181636606	1
Caelo	Sorbitol	18281603	2
Caelo	Sorbitol	18281605	5
Caelo	Sorbitol	18281605P-190624-2	1
Caelo	Sorbitol	18281610	2
Caelo	Sorbitol	19017304	5
Caelo	Sorbitol	19017305	1
Caelo	Sorbitol	19017307	7
Caelo	Sorbitol	19017308	1
Caelo	Sorbitol	19017312	5
Caelo	Sorbitol	192579001	4
Caelo	Sorbitol	192579002	1
Caelo	Sorbitol	192579006	2
Caelo	Sorbitol	192579007	4
Caelo	Sorbitol	200003822010	1
Caelo	Sorbitol	2000322010	1
Caelo	Sorbitol	20003822001	3
Caelo	Sorbitol	20003822005	6
Caelo	Sorbitol	20003822006	1
Caelo	Sorbitol	20003822008	1
Caelo	Sorbitol	20003822010	2
Caelo	Sorbitol	20003822011	1
Caelo	Sorbitol	20003822016	2
Caelo	Sorbitol	20021501	1
Caelo	Sorbitol	2003822012	1
Caelo	Sorbitol	21003580001	2
Caelo	Sorbitol	21003580007	1
Caelo	Sorbitol	21003580008	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sorbitol	225282222169	1
Caelo	Sorbitol	23071201	1
Caelo	Sorbitol	23081401	1
Caelo	Sorbitol	26071402	1
Caelo	Sorbitol	4091401	1
Caelo	Sorbitol	5021307	1
Caelo	Sorbitol	8081402	1
Caesar & Loretz GmbH...	Sorbitol	19017307	1
Caesar & Loretz GmbH...	Sorbitol	192579007	1
Caesar & Loretz GmbH...	Sorbitol	18163607	1
Caesar & Loretz GmbH...	Sorbitol	18281603	1
Caesar & Loretz GmbH...	Sorbitol	19017305	1
Caesar & Loretz GmbH...	Sorbitol	19017307	4
Caesar & Loretz GmbH/Gehe	Sorbitol	19017307	2
Caesar & Loretz GmbH/Gehe	Sorbitol	19017312	1
Caesar & Loretz GmbH/Gehe	Sorbitol	192579007	1
Caesar & Loretz GmbH/Gehe	Sorbitol	20003822008	2
Caesar & Loretz GmbH...	Sorbitol	19017302	2
Caesar & Loretz GmbH...	Sorbitol	19017308	5
Caesar & Loretz GmbH...	Sorbitol	192579002	1
Caesar & Loretz GmbH	Sorbitol	18163606	2
Caesar & Loretz GmbH	Sorbitol	18163607	1
Caesar & Loretz GmbH	Sorbitol	18281602	3
Caesar & Loretz GmbH	Sorbitol	18281605	4
Caesar & Loretz GmbH	Sorbitol	19017302	1
Caesar & Loretz GmbH	Sorbitol	19017304	1
Caesar & Loretz GmbH	Sorbitol	19017307	2
Caesar & Loretz GmbH	Sorbitol	19017312	4
Caesar & Loretz GmbH	Sorbitol	192579002	2
Caesar & Loretz GmbH	Sorbitol	192579004	2
Caesar & Loretz GmbH	Sorbitol	192579006	3
Caesar & Loretz GmbH	Sorbitol	20003822001	2
Caesar & Loretz GmbH	Sorbitol	20003822010	1
Caesar & Loretz GmbH	Sorbitol	21003580008	4
Caesar & Loretz GmbH	Sorbitol	21003580009	1
Caesar u. Loretz GmbH	Sorbitol	20003822006	1
EuRho/Anzag	Sorbitol	3518E-02298	1
EuRho/Anzag	Sorbitol	4712I-02298	1
eurho	Sorbitol	1301019-01	1
EuRho	Sorbitol	161001802	1
Euro OTC	Sorbitol		1
Euro OTC	Sorbitol	1301019-01	3
Euro OTC	Sorbitol	1311034-01	2
Euro OTC	Sorbitol	1404007-01	2
Euro OTC	Sorbitol	1406014-01	1
Euro OTC	Sorbitol	1501048-01	4
Euro OTC	Sorbitol	1506052-01	4
Euro OTC	Sorbitol	150652-01	1
Euro OTC	Sorbitol	1512016-01	4
Euro OTC	Sorbitol	1604007-01	4
Euro OTC	Sorbitol	1610018-01	16
Euro OTC	Sorbitol	1610018-02	3
Euro OTC	Sorbitol	1610018-03	8
Euro OTC	Sorbitol	1810010-01	2
Euro OTC	Sorbitol	1810010-02	2
Euro OTC	Sorbitol	2008016-01	2
Euro OTC	Sorbitol	2008016-02	1
Euro OTC	Sorbitol	200816-01	1
Euro OTC	Sorbitol	2108021-01	1
Euro OTC	Sorbitol	3217M-02298	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Sorbitol	3617I-02298	1
Euro OTC	Sorbitol	700476	1
Fagron	Sorbitol		1
Fagron	Sorbitol	11I09-N11	1
Fagron	Sorbitol	12E30-N24	3
Fagron	Sorbitol	12J15-N01	1
Fagron	Sorbitol	12L17-N12	3
Fagron	Sorbitol	13278249	1
Fagron	Sorbitol	13D08-N27	1
Fagron	Sorbitol	13E07-B40	2
Fagron	Sorbitol	13G04-N04	1
Fagron	Sorbitol	14E21-B02	1
Fagron	Sorbitol	M721140	1
Fagron	Sorbitol	M721140/12L17-N12	1
Gatt-Koller / Phoenix	Sorbitol	1718/0513	1
Gatt-Koller / Phoenix	Sorbitol	1718/05134013	1
Gehe 01.09.2014	Sorbitol	13278217	1
GEHE 28.11.2014	Sorbitol	13278245	1
GEHE	Sorbitol	16353108	1
Gehe	Sorbitol	18163606	1
GEHE	Sorbitol	19017305	1
Gehe	Sorbitol	21003580009	1
Gehe	Sorbitol	22003595005	1
Gehe	Sorbitol	22003595007	1
Gehe	Sorbitol	22003595008	1
Hänseler	Sorbitol		1
Herba ACM	Sorbitol	22J01085	1
Jenne	Sorbitol	22003595008	1
L10	Sorbitol	16353108	1
L12	Sorbitol	17140904	3
Merck	Sorbitol	13D08-N27	1
Noweda/ Ichthyol	Sorbitol	1512016-01	1
Noweda	Sorbitol	17140903	1
Noweda	Sorbitol	22003595008	1
Phoenix 12.08.2013	Sorbitol	12249108	1
PHÖNIX	Sorbitol	18281603	1
phönix	Sorbitol	21003580002	1
Sana	Sorbitol	18281603	1
Sanacorp	Sorbitol	1610018-01	1
Sanacorp	Sorbitol	16353107	1
siehe Protokoll	Sorbitol	15208310	1
Spangro 17.05.19	Sorbitol	17140902	1

- 235 608 spectra from 1515 *Apo-Ident* customers from a total of 49 107 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sorbitol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sorbitol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	680	0	201 404
Type C	0	459	0	235 608

The substance/substance group *Sorbitol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.1176 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 98.6928 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21485	21834	6.05	90.97
21834	21834	0.00	95.64
22293	22293	0.00	89.03
22539	22539	0.00	88.60
22847	21834	3.13	91.92
22849	22849	0.00	88.85
23028	23028	0.00	96.66
23442	21834	5.76	96.72
25226	25226	0.00	110.16

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sotalol hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	22656-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sotalol hydrochloride; Sotaloli hydrochloridum

Special notes

When selecting the *Sotalol hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sotalol hydrochloride	3	1	1

Second-stage model

For differentiation of the substance/substance group *Sotalol hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sotalol hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	135.71	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sotalol hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sotalol hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sotalol hydrochloride	20000112	25199	40	20200210*
Caelo	Sotalol hydrochloride	24002039	27442	40	20241121*
Caelo	Sotalol hydrochloride	24002039	27442SI	20	20241121*
Fagron	Sotalol hydrochloride	21E21-B04-218998	26324	40	20210702
Fagron	Sotalol hydrochloride	21E21-B04-218998	26324SI	20	20210702

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 160 spectra of 5 reference samples from the substance/substance group *Sotalol hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 802 spectra from a total of 2839 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Sotalol hydrochloride*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Inresa	Sotalol hydrochloride	369-MC	22656	40

- 202 044 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Sotalol hydrochloride*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Kehr	Sotalol hydrochloride	21001470007	1

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sotalol hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sotalol hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	160	0	152 802
Type B	0	40	0	202 044
Type C	0	1	0	236 066

The substance/substance group *Sotalol hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25199	25199	0.00	222.44
26324	27442	4.51	222.85
27442	27442	0.00	221.63

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Soy lecithin (instant form)**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20539-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Soy lecithin (instant form); Lecithinum e sojae plv.

Special notes

When selecting the *Soy lecithin (instant form)* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Soy lecithin (instant form)	5	2	40

Second-stage model

For differentiation of the substance/substance group *Soy lecithin (instant form)* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Soy lecithin (instant form)* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Mupirocin calcium	69.50	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Soy lecithin (instant form)* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Soy lecithin (instant form)*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Soy lecithin (instant form)	13030504	20985	40	1404399
Caelo	Soy lecithin (instant form)	13279813	21523	40	20130903
Caelo	Soy lecithin (instant form)	17118101	23370	40	20170620
Caelo	Soy lecithin (instant form)	17118101	23445	40	20170620
Caelo	Soy lecithin (instant form)	191879	24749	40	20190712*
Caelo	Soy lecithin (instant form)	20002522003	25521	40	20200924

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 240 spectra of 6 reference samples from the substance/substance group *Soy lecithin (instant*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

form). These samples are listed above in the *calibration samples* section. The reference samples come from 5 different batches.

- 152 722 spectra from a total of 2837 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 2 reference samples from the substance/substance group *Soy lecithin (instant form)*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Soy lecithin (instant form)	173224	24244	40
Caelo	Soy lecithin (instant form)	21001068004	25784	50

- 201 994 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 83 spectra from 46 *Apo-Ident* customers from 44 batches from the substance/substance group *Soy lecithin (instant form)*.

- Among them are spectra of independent samples from 40 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Soy lecithin (instant form)	23000766003	1
Caelo	Soy lecithin (instant form)		1
Caelo	Soy lecithin (instant form)	11371504	1
Caelo	Soy lecithin (instant form)	12139001	3
Caelo	Soy lecithin (instant form)	12139011	3
Caelo	Soy lecithin (instant form)	12139012	1
Caelo	Soy lecithin (instant form)	13030503	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Soy lecithin (instant form)	13030506	1
Caelo	Soy lecithin (instant form)	13279806	1
Caelo	Soy lecithin (instant form)	13279814	1
Caelo	Soy lecithin (instant form)	14196305	1
Caelo	Soy lecithin (instant form)	14281605	1
Caelo	Soy lecithin (instant form)	14281606	2
Caelo	Soy lecithin (instant form)	14281618	4
Caelo	Soy lecithin (instant form)	14281620	1
Caelo	Soy lecithin (instant form)	15262701	4
Caelo	Soy lecithin (instant form)	15262704	4
Caelo	Soy lecithin (instant form)	1526704	1
Caelo	Soy lecithin (instant form)	16223302	4
Caelo	Soy lecithin (instant form)	17081501	2
Caelo	Soy lecithin (instant form)	17118101	1
Caelo	Soy lecithin (instant form)	17118102	1
Caelo	Soy lecithin (instant form)	17118105	2
Caelo	Soy lecithin (instant form)	17118108	1
Caelo	Soy lecithin (instant form)	17322401	3
Caelo	Soy lecithin (instant form)	17322402	1
Caelo	Soy lecithin (instant form)	17322405	5
Caelo	Soy lecithin (instant form)	18282701	3
Caelo	Soy lecithin (instant form)	19009101	3
Caelo	Soy lecithin (instant form)	19009113	1
Caelo	Soy lecithin (instant form)	20000718005	1
Caelo	Soy lecithin (instant form)	21001068003	1
Caelo	Soy lecithin (instant form)	21002621003	1
Caesar & Loretz GmbH Gehe	Soy lecithin (instant form)	21001068004	1
Caesar & Loretz GmbH...	Soy lecithin (instant form)	12139013	1
Caesar & Loretz GmbH...	Soy lecithin (instant form)	20002522003	2
Caesar & Loretz GmbH...	Soy lecithin (instant form)	20000718001	1
Caesar & Loretz GmbH...	Soy lecithin (instant form)	20000718005	1
Caesar & Loretz GmbH...	Soy lecithin (instant form)	19009110	1
Caesar & Loretz GmbH...	Soy lecithin (instant form)	19009107	1
Caesar & Loretz GmbH	Soy lecithin (instant form)	14281603	1
Caesar & Loretz GmbH	Soy lecithin (instant form)	19009103	2
Caesar & Loretz GmbH	Soy lecithin (instant form)	19187901	2
Caesar &Loretz GmbH	Soy lecithin (instant form)	13030503	1
Caesar &Loretz GmbH	Soy lecithin (instant form)	13279813	1
Gehe	Soy lecithin (instant form)	19187901	1
Gehe	Soy lecithin (instant form)	21002621003	1
INTR/ Sana	Soy lecithin (instant form)	16223302	1
Sanacorp	Soy lecithin (instant form)	14196305	1
Sanacorp	Soy lecithin (instant form)	17322405	1
siehe WE-Prüfprotokoll	Soy lecithin (instant form)	31/14	1

- 235 984 spectra from 1515 *Apo-Ident* customers from a total of 49 216 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Soy lecithin (instant form)* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Soy lecithin (instant form)* and it was evaluated how many matches (positive) and rejections (negative) were correct or

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	240	0	152 722
Type B	0	90	0	201 994
Type C	0	83	0	235 984

The substance/substance group *Soy lecithin (instant form)* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 93.3333 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 92.7711 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20985	20985	0.00	124.60
21523	20985	49.21	126.57
23370	20985	31.45	126.46
23445	20985	36.48	127.30
24749	24749	0.00	124.08
25521	20985	68.27	128.19

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Spironolactone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21032-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Spironolactone; Spironolactonum

Special notes

When selecting the *Spironolactone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Spironolactone	9	15	231

Second-stage model

For differentiation of the substance/substance group *Spironolactone* the following second-stage model is used:

- Submodel 05

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Spironolactone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	104.86	–
⋮	⋮	⋮
Progesterone	>50	62.85
Testosterone propionate	>50	66.04
Povidone iodine	>50	76.66
Fusidic acid	>50	92.10
Ubidecarenone	>50	136.83
Povidone	>50	151.96

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Spironolactone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Spironolactone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Spironolactone	14378715	22385	40	20150211
Caelo	Spironolactone	160773	22444	60	20160415*
Caelo	Spironolactone	190158	24548	40	20190308*
Caelo	Spironolactone	20001838	25213	40	20200617*
Euro OTC	Spironolactone	1212034-01	21032	50	1403151
Euro OTC	Spironolactone	1212034-01	21076	42	20130215
Euro OTC	Spironolactone	1602006	22369	45	20160309*
Euro OTC	Spironolactone	2006012	25311	40	20200821*
Euro OTC	Spironolactone	2006012	25311SI	33	20200821*
Fagron	Spironolactone	15G22-B10-311159	22386	40	20150728
Fagron	Spironolactone	16E20-B06-322016	22942	40	20160531

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 470 spectra of 11 reference samples from the substance/substance group *Spironolactone*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 492 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 736 spectra of 21 reference samples from the substance/substance group *Spironolactone*.

- Among them are spectra of independent samples from 15 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Spironolactone	16077305	22954	40
Caelo	Spironolactone	171165	23327	40
Caelo	Spironolactone	172432	23660	40
Caelo	Spironolactone	182080	24391	40
Caelo	Spironolactone	191979	24748	40
Caelo	Spironolactone	22000904013	26739	40
Euro OTC	Spironolactone	1612002	22909	40
Euro OTC	Spironolactone	1711013	23888	40
Euro OTC	Spironolactone	1809020	24324	40
Euro OTC	Spironolactone	1907001	24782	40
Euro OTC	Spironolactone	2203010	26086	40
Fagron	Spironolactone	22B07-B14-227278	26543	40
Fagron	Spironolactone	120A20240801	BR20035	40
Fagron	Spironolactone	120A20240802	BR20036	40
Fagron	Spironolactone	10A20240801	BR20037SI	20
Caelo	Spironolactone	22000904013	26739SI	31
Euro OTC	Spironolactone	2203010	26086SI	10
Fagron	Spironolactone	22B07-B14-227278	26543SI	35
Fagron	Spironolactone	120A20240801	BR20035SI	20
Fagron	Spironolactone	120A20240802	BR20036SI	20
Fagron	Spironolactone	120A20240801	BR20037	40

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 348 spectra from a total of 4030 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1279 spectra from 468 *Apo-Ident* customers from 241 batches from the substance/substance group *Spironolactone*.

- Among them are spectra of independent samples from 231 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Spironolactone		1
	Spironolactone	22000904001	2
	Spironolactone	22000904002	1
	Spironolactone	22000904007	2
	Spironolactone	22000904008	6
	Spironolactone	22000904011	1
	Spironolactone	22000904012	5
	Spironolactone	22000904013	7
	Spironolactone	22000904015	12
	Spironolactone	22000904018	2
	Spironolactone	23001294004	1
	Spironolactone	23001294005	8
	Spironolactone	23001294006	2
	Spironolactone	24000134003	1
AHD 23.07.2020	Spironolactone	190158003	1
AHD	Spironolactone	22000904008	1
AHD	Spironolactone	22000904012	1
AHD	Spironolactone	23001294005	1
AHD	Spironolactone	24000134003	1
Alliance Healthcare	Spironolactone	12049119	1
Alliance Healthcare	Spironolactone	12049129	1
Alliance	Spironolactone	22000904018	1
Alliance	Spironolactone	24000134003	1
Anzag	Spironolactone	191163002	2
Anzag	Spironolactone	20003886003	2
Anzag	Spironolactone	21000085007	1
apomix	Spironolactone	16077320	1
Caelo	Spironolactone		1
Caelo	Spironolactone	10159914	1
Caelo	Spironolactone	1090216	1
Caelo	Spironolactone	10H24-N10	1
Caelo	Spironolactone	11042602	1
Caelo	Spironolactone	11042607	1
Caelo	Spironolactone	1110917/16077320	1
Caelo	Spironolactone	11G28-N03	1
Caelo	Spironolactone	12049103	1
Caelo	Spironolactone	12049105	2
Caelo	Spironolactone	12049109	1
Caelo	Spironolactone	12049110	2
Caelo	Spironolactone	12049118	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Spironolactone	12049123	3
Caelo	Spironolactone	12049130	4
Caelo	Spironolactone	13124303	7
Caelo	Spironolactone	13124304	7
Caelo	Spironolactone	13124309	6
Caelo	Spironolactone	13124314	2
Caelo	Spironolactone	13124315	6
Caelo	Spironolactone	13124317	3
Caelo	Spironolactone	13124320	3
Caelo	Spironolactone	13124321	2
Caelo	Spironolactone	131243315	1
Caelo	Spironolactone	1314309	1
Caelo	Spironolactone	13190309	3
Caelo	Spironolactone	140202901	1
Caelo	Spironolactone	1437807	1
Caelo	Spironolactone	1437815	1
Caelo	Spironolactone	14378701	2
Caelo	Spironolactone	14378702	4
Caelo	Spironolactone	14378703	1
Caelo	Spironolactone	14378709	4
Caelo	Spironolactone	14378710	5
Caelo	Spironolactone	14378715	8
Caelo	Spironolactone	14378717	3
Caelo	Spironolactone	14378718	9
Caelo	Spironolactone	14378719	1
Caelo	Spironolactone	14378721	2
Caelo	Spironolactone	1438721	1
Caelo	Spironolactone	1496810000858	1
Caelo	Spironolactone	150401601	1
Caelo	Spironolactone	15G22-B10	1
Caelo	Spironolactone	160773	1
Caelo	Spironolactone	16077302	16
Caelo	Spironolactone	16077303	17
Caelo	Spironolactone	16077305	10
Caelo	Spironolactone	16077306	8
Caelo	Spironolactone	16077307	1
Caelo	Spironolactone	16077309	7
Caelo	Spironolactone	1607731	1
Caelo	Spironolactone	16077311	14
Caelo	Spironolactone	16077312	20
Caelo	Spironolactone	16077312/1230817	1
Caelo	Spironolactone	16077316	1
Caelo	Spironolactone	16077319	5
Caelo	Spironolactone	16077320	11
Caelo	Spironolactone	16077324	1
Caelo	Spironolactone	16077325	20
Caelo	Spironolactone	16077326	17
Caelo	Spironolactone	161200201	1
Caelo	Spironolactone	16A14-B05-317123	1
Caelo	Spironolactone	16D15-B06-320903	1
Caelo	Spironolactone	16H20-B06-322016	1
Caelo	Spironolactone	17116501	1
Caelo	Spironolactone	171165012	1
Caelo	Spironolactone	17116502	9
Caelo	Spironolactone	17H16-B05-341740	1
Caelo	Spironolactone	17H16-B05-344771	1
Caelo	Spironolactone	18004803	12
Caelo	Spironolactone	18004902	3
Caelo	Spironolactone	18004904	20
Caelo	Spironolactone	18004908	12

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Spironolactone	18004912	1
Caelo	Spironolactone	18004913	4
Caelo	Spironolactone	18004915	13
Caelo	Spironolactone	18004915P-190531-5	1
Caelo	Spironolactone	18004917	22
Caelo	Spironolactone	18004917P-190604-1	1
Caelo	Spironolactone	18004919	1
Caelo	Spironolactone	18004920	17
Caelo	Spironolactone	18004922	1
Caelo	Spironolactone	180208003	1
Caelo	Spironolactone	18205004	1
Caelo	Spironolactone	18208003	12
Caelo	Spironolactone	18208004	11
Caelo	Spironolactone	18208005	1
Caelo	Spironolactone	18208008	15
Caelo	Spironolactone	18208008P-191007-1	1
Caelo	Spironolactone	18208010	12
Caelo	Spironolactone	18A24-B03-348018	5
Caelo	Spironolactone	190158001	15
Caelo	Spironolactone	190158003	1
Caelo	Spironolactone	190158004	1
Caelo	Spironolactone	19015801	1
Caelo	Spironolactone	19015802	1
Caelo	Spironolactone	190158022	1
Caelo	Spironolactone	19015803	23
Caelo	Spironolactone	19015804	16
Caelo	Spironolactone	19015805	3
Caelo	Spironolactone	19015809	8
Caelo	Spironolactone	19015809P-200507-2	1
Caelo	Spironolactone	1907001-01	2
Caelo	Spironolactone	191163001	9
Caelo	Spironolactone	191163002	27
Caelo	Spironolactone	191163003	1
Caelo	Spironolactone	191163004	8
Caelo	Spironolactone	191163008	13
Caelo	Spironolactone	20003605013	1
Caelo	Spironolactone	2000386003	1
Caelo	Spironolactone	20003886003	30
Caelo	Spironolactone	20003886004	2
Caelo	Spironolactone	20003886005	8
Caelo	Spironolactone	2013U-03249	1
Caelo	Spironolactone	210000085007	1
Caelo	Spironolactone	21000085001	2
Caelo	Spironolactone	21000085002	15
Caelo	Spironolactone	210000850022	1
Caelo	Spironolactone	21000085004	12
Caelo	Spironolactone	21000085006	1
Caelo	Spironolactone	21000085007	12
Caelo	Spironolactone	21000085008	6
Caelo	Spironolactone	21000085009	20
Caelo	Spironolactone	21000085010	11
Caelo	Spironolactone	21000085012	2
Caelo	Spironolactone	21000085015	11
Caelo	Spironolactone	21000085017	11
Caelo	Spironolactone	21000085018	3
Caelo	Spironolactone	2100008508	1
Caelo	Spironolactone	2100008509	2
Caelo	Spironolactone	210000855007	1
Caelo	Spironolactone	2100085007	1
Caelo	Spironolactone	2100085017	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Spironolactone	22000904001	12
Caelo	Spironolactone	22000904002	14
Caelo	Spironolactone	22000904008	2
Caelo	Spironolactone	22000904012	2
Caelo	Spironolactone	2200090404002	1
Caelo	Spironolactone	22121701	1
Caelo	Spironolactone	5013Q-03249	1
Caeol/ Noweda	Spironolactone	16077305	2
Caeol/Noweda	Spironolactone	16077303	1
Caeol/Noweda	Spironolactone	18208008	1
Caesar & Loretz GmbH...	Spironolactone	18004915	1
Caesar & Loretz GmbH...	Spironolactone	18004920	1
Caesar & Loretz GmbH...	Spironolactone	190158001	3
Caesar & Loretz GmbH...	Spironolactone	22000904002	1
Caesar & Loretz GmbH...	Spironolactone	18208010	2
Caesar & Loretz GmbH...	Spironolactone	21000085010	1
Caesar & Loretz GmbH...	Spironolactone	22000904001	1
Caesar & Loretz GmbH...	Spironolactone	19015803	1
Caesar & Loretz GmbH/AHD	Spironolactone	21000085002	1
Caesar & Loretz GmbH/AHD	Spironolactone	21000085010	2
Caesar & Loretz GmbH...	Spironolactone	191163008	1
Caesar & Loretz GmbH/Gehe	Spironolactone	190158001	2
Caesar & Loretz GmbH/Gehe	Spironolactone	19015803	2
Caesar & Loretz GmbH/Gehe	Spironolactone	19015804	1
Caesar & Loretz GmbH/Gehe	Spironolactone	191163004	1
Caesar & Loretz GmbH/GEHE	Spironolactone	191163008	1
Caesar & Loretz GmbH/GEHE	Spironolactone	21000085002	1
Caesar & Loretz GmbH/Gehe	Spironolactone	21000085007	1
Caesar & Loretz GmbH/Kehr	Spironolactone	22000904001	2
Caesar & Loretz GmbH...	Spironolactone	18208010	5
Caesar & Loretz GmbH...	Spironolactone	19015804	1
Caesar & Loretz GmbH...	Spironolactone	19015809	1
Caesar & Loretz GmbH...	Spironolactone	191163004	1
Caesar & Loretz GmbH...	Spironolactone	21000085007	1
Caesar & Loretz GmbH...	Spironolactone	18208010	1
Caesar & Loretz GmbH...	Spironolactone	190158004	1
Caesar & Loretz GmbH...	Spironolactone	19015803	2
Caesar & Loretz GmbH...	Spironolactone	20003886003	1
Caesar & Loretz GmbH...	Spironolactone	21000085004	1
Caesar & Loretz GmbH...	Spironolactone	18004915	1
Caesar & Loretz GmbH	Spironolactone	12049129	1
Caesar & Loretz GmbH	Spironolactone	18004917	1
Caesar & Loretz GmbH	Spironolactone	18004920	2
Caesar & Loretz GmbH	Spironolactone	18208003	4
Caesar & Loretz GmbH	Spironolactone	18208004	1
Caesar & Loretz GmbH	Spironolactone	18208008	4
Caesar & Loretz GmbH	Spironolactone	18208010	1
Caesar & Loretz GmbH	Spironolactone	190158001	7
Caesar & Loretz GmbH	Spironolactone	190158004	2
Caesar & Loretz GmbH	Spironolactone	19015803	2
Caesar & Loretz GmbH	Spironolactone	19015804	11
Caesar & Loretz GmbH	Spironolactone	19015809	3
Caesar & Loretz GmbH	Spironolactone	191163001	2
Caesar & Loretz GmbH	Spironolactone	191163002	7
Caesar & Loretz GmbH	Spironolactone	191163004	3
Caesar & Loretz GmbH	Spironolactone	191163008	6
Caesar & Loretz GmbH	Spironolactone	20003886002	1
Caesar & Loretz GmbH	Spironolactone	20003886003	4
Caesar & Loretz GmbH	Spironolactone	20003886004	1
Caesar & Loretz GmbH	Spironolactone	20003886005	8

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Spironolactone	21000085001	3
Caesar & Loretz GmbH	Spironolactone	21000085002	5
Caesar & Loretz GmbH	Spironolactone	21000085004	7
Caesar & Loretz GmbH	Spironolactone	21000085006	2
Caesar & Loretz GmbH	Spironolactone	21000085007	7
Caesar & Loretz GmbH	Spironolactone	21000085008	6
Caesar & Loretz GmbH	Spironolactone	21000085009	4
Caesar & Loretz GmbH	Spironolactone	21000085010	10
Caesar & Loretz GmbH	Spironolactone	21000085015	6
Caesar & Loretz GmbH	Spironolactone	21000085017	7
Caesar & Loretz GmbH	Spironolactone	21000085018	2
Caesar & Loretz GmbH	Spironolactone	22000904001	10
Caesar & Loretz GmbH	Spironolactone	22000904002	3
Caesar & Loretz GmbH	Spironolactone	22000904004	1
Caesar & Loretz GmbH	Spironolactone	22000904008	1
Caesar & Loretz GmbH	Spironolactone	22000904018	1
Caesar & Loretz GmbH...	Spironolactone	20003886005	1
Caesar u Loretz	Spironolactone	12049119	1
Caesar u. Loretz / G...	Spironolactone	18208010	1
Caesar und Loretz GmbH	Spironolactone	191163008	1
Caesar&Loretz GmbH	Spironolactone	19015804	1
Caesar&loretz,Anzag	Spironolactone	13124309	1
Caesar&loretz,Phoenix	Spironolactone	11042603	1
Caesar&loretz,Phoenix	Spironolactone	11042613	1
Caesar/Lorenz	Spironolactone	13124303	1
Cealo/Gehe	Spironolactone	18004904	2
EuRho / Noweda	Spironolactone	200612-01	1
Eurho/Anzag	Spironolactone	190700101	1
EuRho	Spironolactone	1101013-01	1
Euro OTC	Spironolactone	1000403502	1
Euro OTC	Spironolactone	1004035	1
Euro OTC	Spironolactone	1101013-01	1
Euro OTC	Spironolactone	1212034-01	6
Euro OTC	Spironolactone	1402029-01	1
Euro OTC	Spironolactone	14378721	1
Euro OTC	Spironolactone	1504016-01	3
Euro OTC	Spironolactone	16020006-01	1
Euro OTC	Spironolactone	1602006-01	5
Euro OTC	Spironolactone	1602006-02	1
Euro OTC	Spironolactone	1612002_01	1
Euro OTC	Spironolactone	161200201	1
Euro OTC	Spironolactone	1612002-01	5
Euro OTC	Spironolactone	16E20-B06-322016	1
Euro OTC	Spironolactone	171101301	1
Euro OTC	Spironolactone	1711013-01	12
Euro OTC	Spironolactone	180902001	1
Euro OTC	Spironolactone	1809020-01	5
Euro OTC	Spironolactone	1809020-02	1
Euro OTC	Spironolactone	190700-01	1
Euro OTC	Spironolactone	1907001-01	9
Euro OTC	Spironolactone	2006012-01	5
Euro OTC	Spironolactone	3513E-03249	1
Fagron	Spironolactone		1
Fagron	Spironolactone	10C29-N09	1
Fagron	Spironolactone	10H24-N10	1
Fagron	Spironolactone	12/17-n01	1
Fagron	Spironolactone	12/17-N01	1
Fagron	Spironolactone	12I17-N01	1
Fagron	Spironolactone	12J15-N04	1
Fagron	Spironolactone	13D12-N08	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Spironolactone	13G03-N09	1
Fagron	Spironolactone	13G16-B08	1
Fagron	Spironolactone	13G16-B08-288051	1
Fagron	Spironolactone	14B20B06294618	1
Fagron	Spironolactone	14B20-B06-294618	5
Fagron	Spironolactone	14j02-b02-303621	1
Fagron	Spironolactone	14J02-B02-303621	5
Fagron	Spironolactone	14J02-B02-303622	1
Fagron	Spironolactone	14J02-B303621	1
Fagron	Spironolactone	15G22-B10-311159	2
Fagron	Spironolactone	16A14-B05	1
Fagron	Spironolactone	16A14-B05-317123	1
Fagron	Spironolactone	16A14-B05-525187	1
Fagron	Spironolactone	16D15-B06-320903	1
Fagron	Spironolactone	16E20-B06-322016	1
Fagron	Spironolactone	16E20-B06-325478	2
Fagron	Spironolactone	16I06-B04	1
Fagron	Spironolactone	16I06B04329443	1
Fagron	Spironolactone	16I06-B04-329443	1
Fagron	Spironolactone	17116502	1
Fagron	Spironolactone	17E22-B11-335454	2
Fagron	Spironolactone	17E22-B11-335455	2
Fagron	Spironolactone	17H16-B05	2
Fagron	Spironolactone	17H16-B05-341739	2
Fagron	Spironolactone	17H16-B05-344771	3
Fagron	Spironolactone	18208003	1
Fagron	Spironolactone	18A24-B03	1
Fagron	Spironolactone	18A24-B03-349548	6
Fagron	Spironolactone	18A24-B03-354314	2
Fagron	Spironolactone	18G12-B01-356145	3
Fagron	Spironolactone	19C29-B06-191465	3
Fagron	Spironolactone	19H23-B06-194244	1
Fagron	Spironolactone	19H23-B06-194245	1
Fagron	Spironolactone	19H23-B06-194567	1
Fagron	Spironolactone	19H23-B06-194569	2
Fagron	Spironolactone	19H23-B06-194245	1
Fagron	Spironolactone	2006012-01	2
Fagron	Spironolactone	20B24-B04	2
Fagron	Spironolactone	20B24-B04-200519	1
Fagron	Spironolactone	20B24-B04-200520	5
Fagron	Spironolactone	20H19-B01-202267	2
Fagron	Spironolactone	20H19-B01-213618	2
Fagron	Spironolactone	21H27-B05-217974	3
Fagron	Spironolactone	21H27-B05-222385	1
Fagron	Spironolactone	2415E-03249	1
Fagron	Spironolactone	2517Q03249	1
Fagron	Spironolactone	2918E-03249	1
Fagron	Spironolactone	80616-7	1
Fagron	Spironolactone	B01-2022607	1
Fagron	Spironolactone	B04-2005109	1
Fagron	Spironolactone	B04-2005200	1
Fagron	Spironolactone	eln170404	1
Fagron	Spironolactone	SA1063	2
Fiebig	Spironolactone	191163001	1
Fiebig	Spironolactone	19h23-b06-194567	1
Fiebig	Spironolactone	B06-1945607	1
Gehe	Spironolactone	12049105	1
Gehe	Spironolactone	13D12-N08	1
GEHE	Spironolactone	16077325	1
gehe	Spironolactone	17E22-B11-335455	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Spironolactone	17H16-B05-341740	1
Gehe	Spironolactone	18208003	1
Gehe	Spironolactone	19015803	1
Gehe	Spironolactone	191163008	1
Gehe	Spironolactone	21000085010	1
Jenne	Spironolactone	14378715	1
Kehr	Spironolactone	22000904008	1
Kehr	Spironolactone	22000904012	1
Noweda/ Caesar&Loren...	Spironolactone	18208008	1
Noweda	Spironolactone	1101013-0	1
Noweda	Spironolactone	14378710	1
Noweda	Spironolactone	1504016-01	1
Noweda	Spironolactone	1602006-01	1
Noweda	Spironolactone	1612002-01	1
noweda	Spironolactone	16A14-B05-525187	1
Noweda	Spironolactone	19H23-B06-194245	1
Noweda	Spironolactone	21000085017	1
Noweda	Spironolactone	22000904012	1
Noweda	Spironolactone	22000904013	2
Noweda	Spironolactone	2203010-01	1
Noweeda	Spironolactone	22000904005	1
Phoenix	Spironolactone	1612002-01	2
Phoenix	Spironolactone	18208008	1
Phoenix	Spironolactone	18A24-B03-354314	1
Phoenix	Spironolactone	19C29-B06-191465	1
Phoenix	Spironolactone	19H23-B06-1942405	2
Phönix	Spironolactone	1101013-03	1
Phönix	Spironolactone	17H16-B05-344771	1
Phönix	Spironolactone	1809020-01	2
Phönix	Spironolactone	18208003	1
Phönix	Spironolactone	18208004	1
Phönix	Spironolactone	191163002	3
Phönix	Spironolactone	20003886005	2
Phönix	Spironolactone	2006012-01	1
Phönix	Spironolactone	21000085007	1
Phönix	Spironolactone	2203010-01	2
Sanacorp/Phoenix	Spironolactone	13124315	2
Sanacorp	Spironolactone	11042612	1
Sanacorp	Spironolactone	12049103	2
Sanacorp	Spironolactone	12049130	1
Sanacorp	Spironolactone	1212034-01	1
Sanacorp	Spironolactone	13124304	1
Sanacorp	Spironolactone	13124315	1
Sanacorp	Spironolactone	16077325	2
Sanacorp	Spironolactone	18004913	1
Sanacorp	Spironolactone	18208004	1
Sanacorp	Spironolactone	19H23-B06-194567	1
Sanacorp	Spironolactone	20003886005	1
Sanacorp	Spironolactone	22000904018	1
Sanacorp	Spironolactone	23001294006	1
Sanacorp	Spironolactone	9330610	1
WE Phönix 25.11..201...	Spironolactone	16077303	1
Zhejiang Langhua /Phönix	Spironolactone	18004917	2
Zhejiang Langhua /Phönix	Spironolactone	18208003	1
Zhejiang Langhua Pha...	Spironolactone	Q3312	1
Zhejiang/Phoenix	Spironolactone	OT00E1902002	1

- 234 788 spectra from 1515 *Apo-Ident* customers from a total of 49 022 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are docu-

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

mented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Spironolactone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Spironolactone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	470	0	152 492
Type B	0	736	0	201 348
Type C	0	1177	102	234 788

The substance/substance group *Spironolactone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7234 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.1848 %)
Type C	100.0000 % (> 99.9007 %)	92.0250 % (> 91.7905 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21032	21032	0.00	122.45
21076	21032	4.34	118.67
22369	22369	0.00	127.05
22385	22369	6.66	116.97
22386	22444	5.26	116.88
22444	22444	0.00	117.29
22942	22369	3.81	121.09
24548	24548	0.00	116.91
25213	25213	0.00	112.40
25311	25311	0.00	123.57

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Starch**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20790-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Starch; Amylum Maydis; Amylum oryzae; Corn starch; Potato starch; Rice starch; Solani amylum; SyrSpend® SF Alka; SyrSpend® SF pH4; SyrSpend® SF pH4 neo (Maize starch); Tritici amylum; Wheat starch

Special notes

When selecting the *Starch* substance/substance group, the following information is displayed to the user:

- Advice for the identification of SyrSpend® SF Alka: Please shake the sample before the measurement to ensure an even particle distribution.

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Starch	39	28	521

Second-stage model

For differentiation of the substance/substance group *Starch* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Starch* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Maltodextrin	27.19	21.32
Acacia, dried dispersion	32.16	19.94
Sodium cromoglicate	49.44	–
Polymyxin B sulfate	74.98	31.26
⋮	⋮	⋮
Carmellose sodium	>50	15.48
Colistin sulfate	>50	27.30
Calcium glycerophosphate	>50	34.10
Cyanocobalamin	>50	42.15
Amphotericin B	>50	42.30
Bacitracin	>50	48.19
Riboflavin	>50	58.24
Selenium yeast	>50	61.71
Tosylchloramide sodium	>50	70.62
Oxalic acid	>50	74.74
Fructose	>50	75.79
Calcium pantothenate	>50	77.29
Nystatin	>50	78.88
Gelatine, white	>50	95.04
Hyoscine hydrobromide	>50	103.52
alpha-tocopheryl acetate dry concentrate	>50	117.17
Estradiol hemihydrate	>50	124.00
Triamcinolone	>50	130.27
Methylcobalamin	>50	153.73
Estriol	>50	165.95

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Starch* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Starch*:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Corn starch	13154914	21827	60	20130529
Caelo	Corn starch	161385	22450	60	20160621*
Caelo	Corn starch	182748	24361	40	20181031*
Caelo	Corn starch	24001513	27324	40	20240722*
Klenk	Corn starch	0064A200427-01	25383	40	20200515
Caelo	Potato starch	12360213	20996	40	1403494
Caelo	Potato starch	14033815	21965	60	20140207
Caelo	Potato starch	161237	22449	60	20160621*
Caelo	Potato starch	24001388	27321	40	20240722*
Klenk	Potato starch	0094A170123	23923	40	20170309
Klenk	Potato starch	0094A180919-01	25382	40	20200804
Caelo	Rice starch	12068525	20790	40	20120327
Caelo	Rice starch	16144501	22585	40	20160504
Euro OTC	Rice starch	1912005	25080	40	20200109*
Euro OTC	Rice starch	2101008	25534	40	20210129*
Euro OTC	Rice starch	2107016	25767	50	20210816*
Fagron	Rice starch	16B25-B01-327231	23219	40	20160308
Fagron	Rice starch	16B25-B01-327231	23220	40	AR-17-FG-015298-02
Fagron	SyrSpend® SF Alka	17D11-B04-332593	23448	40	20170505
Fagron	SyrSpend® SF Alka	17D11-B04-332593	23449	40	20170505
Fagron	SyrSpend® SF Alka	17F14-B02-335945	23750	20	1804106
Fagron	SyrSpend® SF Alka	18B21-B08-347192	24112	40	1809264
Fagron	SyrSpend® SF Alka	18C13-B11-350851	24290	40	20180502
Fagron	SyrSpend® SF Alka	20B25-F06-369913	25363	40	20200424
Fagron	SyrSpend® SF Alka	23B16-F01-384773	27029	40	20230502
Fagron	SyrSpend® SF pH4	15A26-B04-311720	22496	40	1608352
Fagron	SyrSpend® SF pH4	15A26-B04-311720	22497	40	20150223
Fagron	SyrSpend® SF pH4	15A26-B04-305667	22719	40	1701055
Fagron	SyrSpend® SF pH4	19L05-F10-368874	25369	40	20200320
Fagron	SyrSpend® SF pH4	22L20-F03-384076	26613	40	20230124
Fagron	SyrSpend® SF pH4	22L20-F03-384076	26613SI	20	20230124
Fagron	SyrSpend® SF pH4	23H11-F02-385247	27030	40	20231005
Fagron	SyrSpend® SF pH4	23E23-F05-385178	27056	40	20230807
Fagron	SyrSpend® SF pH4 neo (Mai…	21G23-F02-379002	25755	50	2112411
Fagron	SyrSpend® SF pH4 neo (Mai…	23A18-H15-00941	26568	40	20230120
Fagron	SyrSpend® SF pH4 neo (Mai…	23C21-H01-00941	26677	40	20230328
Fagron	SyrSpend® SF pH4 neo (Mai…	23C21-H01-00941	26677SI	20	20230328
Fagron	SyrSpend® SF pH4 neo (Mai…	23K02-H08-00941	27180	40	20231113
Fagron	SyrSpend® SF pH4 neo (Mai…	24B28-H08-00941	27192	40	20240308
Caelo	Wheat starch	14023203	21447	60	AR-16-FG-011433-01
Caelo	Wheat starch	15124707	22246	60	20150527
Caelo	Wheat starch	23002728	27107	40	20240123*
Klenk	Wheat starch	0104A141114	21973	60	20141210
Klenk	Wheat starch	0104A160512	23510	40	20160628

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 1860 spectra of 44 reference samples from the substance/substance group *Starch*. These samples are listed above in the *calibration samples* section. The reference samples come from 39 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 151 102 spectra from a total of 2803 batches from further 477 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1550 spectra of 47 reference samples from the substance/substance group *Starch*.
- Among them are spectra of independent samples from 28 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Corn starch	16138505	23217	40
Caelo	Corn starch	172873	23813	40
Caelo	Corn starch	170474	24037	40
Caelo	Potato starch	15062921	23189	40
Caelo	Potato starch	173003	23811	40
Caelo	Potato starch	20001764	25660	40
Caelo	Potato starch	21004156	26015	30
Caelo	Rice starch	162180	22642	40
Caelo	Rice starch	190169	24551	40
Caelo	Rice starch	190168	24553	40
Caelo	Rice starch	20001724	25661	40
Caelo	Rice starch	23001380	27254	40
Caelo	Rice starch	2405002	27276	40
Euro OTC	Rice starch	2204008	26200	40
Euro OTC	Rice starch	2301042	26596	40
Euro OTC	Rice starch	2309004	26932	40
Fagron	SyrSpend® SF Alka	15H11-B04-311722	22494	40
Fagron	SyrSpend® SF Alka	22B04-F07-381936	26457	40
Fagron	SyrSpend® SF Alka	22K18-F04-38394	27028	40
Fagron	SyrSpend® SF pH4	15H13-B03-314611	23450	40
Fagron	SyrSpend® SF pH4	16J10-B03-330757	23749	40
Fagron	SyrSpend® SF pH4	23B13-F02-384539	26731	40
Fagron	SyrSpend® SF pH4 neo (Mai…	22B04-F01-381138	25936	40
Fagron	SyrSpend® SF pH4 neo (Mai…	23L01-H01-00941	27181	40
Fagron	SyrSpend® SF pH4 neo (Mai…	24A09-H07-00941	27182	40
Caelo	Wheat starch	15421507	23509	40
Caelo	Wheat starch	181200	24014	40
Caelo	Wheat starch	192516	24885	40
Caelo	Corn starch	24001513	27324SI†	20
Caelo	Potato starch	21004156	26015SI	10
Caelo	Potato starch	24001388	27321SI†	20
Euro OTC	Rice starch	2204008	26200SI	20
Euro OTC	Rice starch	2301042	26596SI	20
Euro OTC	Rice starch	2309004	26932SI	20

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	SyrSpend® SF Alka	15H11-B04-311722	22495	40
Fagron	SyrSpend® SF Alka	15H11-B04-311722	22718	40
Fagron	SyrSpend® SF Alka	17F14-B02-335945	23750†	20
Fagron	SyrSpend® SF Alka	15H11-B04-311722	23768	40
Fagron	SyrSpend® SF Alka	22B04-F07-381936	26457SI	20
Fagron	SyrSpend® SF Alka	22K18-F04-38394	27028SI	20
Fagron	SyrSpend® SF Alka	23B16-F01-384773	27029SI†	20
Fagron	SyrSpend® SF pH4	15H13-B03-314611	23451	40
Fagron	SyrSpend® SF pH4	23B13-F02-384539	26731SI	20
Fagron	SyrSpend® SF pH4	23H11-F02-385247	27030SI†	20
Fagron	SyrSpend® SF pH4 neo (Mai…	22B04-F01-381138	25936SI	10
Fagron	SyrSpend® SF pH4 neo (Mai…	23K02-H08-00941	27180SI†	20
Caelo	Wheat starch	23002728	27107SI†	20

- 200 534 spectra from a total of 4010 batches from further 832 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1837 spectra from 490 *Apo-Ident* customers from 538 batches from the substance/substance group *Starch*.
- Among them are spectra of independent samples from 502 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Corn starch	20004426022	1
	Rice starch	20004428022	3
	Rice starch	20004428041	1
	Wheat starch	21002057002	1
	SyrSpend® SF pH4	22109-F01-283384	1
	SyrSpend® SF Alka	22A12-F20-381408	1
	SyrSpend® SF Alka	22A12-F22-382195	4
	SyrSpend® SF Alka	22B04-F06-381564	1
	SyrSpend® SF Alka	22B04-F07-381936	2
	SyrSpend® SF pH4	22I09-F02-383489	1
	SyrSpend® SF pH4	22I09-F03	1
	SyrSpend® SF pH4	22I09-F03-383490	2
	SyrSpend® SF Alka	22J04F02383639	1
	SyrSpend® SF Alka	22J04-F02-383639	2
	SyrSpend® SF Alka	22J04-F06-3636502	3
	SyrSpend® SF Alka	22J04-F06-383652	8
	SyrSpend® SF Alka	22J04-F08-383658	4
	SyrSpend® SF Alka	22J04-F11-383746	5
	SyrSpend® SF Alka	22J31-F01-526993	1
	SyrSpend® SF Alka	22j31-F01-526993	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
	SyrSpend® SF Alka	22J04-F06-383652	1
	SyrSpend® SF pH4	22K08-F02-383826	6
	SyrSpend® SF pH4	22k08-F02-93826	1
	SyrSpend® SF Alka	22K17-F04-384631	1
	SyrSpend® SF Alka	22K17-F05-384376	1
	SyrSpend® SF Alka	22K18-F01-384185	1
	SyrSpend® SF pH4	22L20-F03-384076	2
	Rice starch	23001380003	2
	SyrSpend® SF pH4	23A03-F09-384187	1
	SyrSpend® SF pH4	23A03-F10-384538	1
	SyrSpend® SF Alka	23A18-F07-384725	3
	SyrSpend® SF pH4	23B13-F02-384539	2
	SyrSpend® SF pH4	23B13-F02-3845309	1
	SyrSpend® SF Alka	23B16-F01-384773	3
	SyrSpend® SF Alka	23B16-F02-384774	2
	SyrSpend® SF Alka	23B16-F03-384777	2
	SyrSpend® SF pH4	23E22-F03-384948	1
	SyrSpend® SF pH4	23E23-F05-385116	1
	Corn starch	30502-01	2
	Rice starch	84A180522	1
	SyrSpend® SF Alka	F01-3847703	1
	SyrSpend® SF pH4	F02-2845309	1
	SyrSpend® SF Alka	F0238363009	1
	SyrSpend® SF pH4	F05-3811006	1
	SyrSpend® SF Alka	F07-3819306	1
	SyrSpend® SF pH4 neo (Mai…	H09-0094001	1
AHD	SyrSpend® SF Alka	22J04-F06-383652	2
AHD	SyrSpend® SF Alka	22K17-F05-384376	1
AHD	SyrSpend® SF Alka	23A18-F07-384725	1
AHD	Corn starch	64A170123	1
AHD	Corn starch	64A230502-01	1
Alliance Healthcare	SyrSpend® SF Alka	20G03-F12-374282	1
Alliance	Wheat starch	192516005	1
Anzag 05.03.13 ek: 9,65EUR	Wheat starch	104A120621	2
Anzag	SyrSpend® SF pH4	23E22-F01-384947	1
Bombastus	Potato starch	12214303	2
Bombastus	Corn starch	15310902	1
Bombastus	SyrSpend® SF pH4	18I16-B01-357703	1
Caelo	Rice starch	10061134	2
Caelo	Corn starch	10061146	1
Caelo	Rice starch	10177507	1
Caelo	Rice starch	10177515	1
Caelo	Rice starch	104A120621	1
Caelo	Rice starch	104A141114	3
Caelo	Wheat starch	104A160512	1
Caelo	Wheat starch	104A171122	1
Caelo	Rice starch	11132406	1
Caelo	Wheat starch	11145011	1
Caelo	Wheat starch	11146011	1
Caelo	Wheat starch	1114611	1
Caelo	Corn starch	11179307	2
Caelo	Rice starch	11186026	1
Caelo	Potato starch	11301012	2
Caelo	Wheat starch	11350907	1
Caelo	Wheat starch	11350911	2
Caelo	Rice starch	12166007	3
Caelo	Rice starch	12214303	1
Caelo	Corn starch	12238705	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Rice starch	12238714	1
Caelo	Corn starch	12238715	2
Caelo	Rice starch	12238719	1
Caelo	SyrSpend® SF Alka	12B23-B07-305668	1
Caelo	Rice starch	13005905	2
Caelo	Rice starch	13005908	1
Caelo	Rice starch	13154904	3
Caelo	Rice starch	13154914	2
Caelo	Rice starch	13305103	3
Caelo	Rice starch	13305108	1
Caelo	Rice starch	14011612	3
Caelo	Rice starch	14011621	1
Caelo	Rice starch	14011630	2
Caelo	Rice starch	14023203	3
Caelo	Rice starch	14025710	1
Caelo	Rice starch	14025733	1
Caelo	Rice starch	14025734	1
Caelo	Potato starch	14033815	1
Caelo	Corn starch	14111701	1
Caelo	Rice starch	14301214	3
Caelo	Potato starch	15062912	2
Caelo	Potato starch	15062915	1
Caelo	Rice starch	15118607	1
Caelo	Rice starch	15119011	6
Caelo	Wheat starch	15124707	2
Caelo	Wheat starch	15124710	1
Caelo	Wheat starch	1512477	1
Caelo	Corn starch	15210908	2
Caelo	Corn starch	15310902	5
Caelo	Corn starch	15310903	3
Caelo	Corn starch	15310904	1
Caelo	Corn starch	15310908	3
Caelo	Corn starch	15310909	2
Caelo	Corn starch	15310914	6
Caelo	Wheat starch	15421507	2
Caelo	Rice starch	16101401	1
Caelo	Corn starch	16138505	5
Caelo	Corn starch	16138507	4
Caelo	Rice starch	16144506	1
Caelo	Wheat starch	16162905	3
Caelo	Rice starch	16218002	2
Caelo	Rice starch	16218009	1
Caelo	Rice starch	16218013	1
Caelo	SyrSpend® SF pH4	16J10-B03-330757	1
Caelo	Potato starch	17037404	1
Caelo	Corn starch	17047404	12
Caelo	Rice starch	17173501	2
Caelo	Wheat starch	17183201	1
Caelo	Corn starch	17287302	7
Caelo	Corn starch	17287305	2
Caelo	Corn starch	17287306	1
Caelo	Potato starch	17327201	3
Caelo	Rice starch	17327502	1
Caelo	Rice starch	17327503	2
Caelo	Rice starch	17327506	2
Caelo	Corn starch	17327601	2
Caelo	Wheat starch	18120004	2
Caelo	Wheat starch	18120012	2
Caelo	SyrSpend® SF Alka	18125-B15-357803	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Potato starch	182059005	2
Caelo	Potato starch	18205905	3
Caelo	Corn starch	18274802	9
Caelo	Corn starch	18274804	11
Caelo	Corn starch	18274808	2
Caelo	SyrSpend® SF Alka	18871B06	1
Caelo	SyrSpend® SF pH4	18A22_B05_346147	1
Caelo	SyrSpend® SF Alka	18B21-B08	1
Caelo	SyrSpend® SF Alka	18C13-B11-350851	1
Caelo	SyrSpend® SF Alka	18H01-B12-353473	1
Caelo	SyrSpend® SF pH4	18H30-B02	1
Caelo	SyrSpend® SF Alka	18J25-B15-357803	2
Caelo	Rice starch	190168001	1
Caelo	Rice starch	190168003	5
Caelo	Rice starch	190168004	3
Caelo	Rice starch	19016801	1
Caelo	Rice starch	19016803	8
Caelo	Rice starch	19016805	1
Caelo	Corn starch	1918702	1
Caelo	Corn starch	191878005	3
Caelo	Corn starch	19187802	7
Caelo	Corn starch	19187803	1
Caelo	Wheat starch	192516001	2
Caelo	Wheat starch	192516005	4
Caelo	Corn starch	20000573002	6
Caelo	Potato starch	20003937003	1
Caelo	Corn starch	20004426002	1
Caelo	Corn starch	20004426005	5
Caelo	Corn starch	20004426010	1
Caelo	Corn starch	20004426013	1
Caelo	Corn starch	2000442602	1
Caelo	Rice starch	20004428002	2
Caelo	Rice starch	20004428003	1
Caelo	Rice starch	20004428022	1
Caelo	Rice starch	200613K3	1
Caelo	SyrSpend® SF pH4	20A09-F03-369540	1
Caelo	Wheat starch	21002057001	3
Caelo	Wheat starch	21002057006	1
Caelo	Wheat starch	21002057007	1
Caelo	Rice starch	2212M-01115	1
Caelo	Rice starch	23001380004	1
Caelo	SyrSpend® SF Alka	353473	1
Caelo	Rice starch	64A130304	6
Caelo	Corn starch	64A170123	1
Caelo	Corn starch	64A200427-01	1
Caelo	SyrSpend® SF Alka	720026-000	1
Caelo	Rice starch	9352108	1
Caelo	Potato starch	94A18091901	1
Caesar & Loretz GmbH/AHD	Corn starch	20000573002	1
Caesar & Loretz GmbH...	Wheat starch	192516001	1
Caesar & Loretz GmbH/Gehe	Corn starch	18274808	1
Caesar & Loretz GmbH/Gehe	Corn starch	19187802	2
Caesar & Loretz GmbH/Sana	Wheat starch	21002057001	1
Caesar & Loretz GmbH	Wheat starch	16162908	2
Caesar & Loretz GmbH	Rice starch	17327510	1
Caesar & Loretz GmbH	Wheat starch	18120012	1
Caesar & Loretz GmbH	Corn starch	18274802	1
Caesar & Loretz GmbH	Corn starch	18274804	2
Caesar & Loretz GmbH	Rice starch	190168004	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Wheat starch	192516005	1
Caesar & Loretz GmbH	Corn starch	20000573002	2
Caesar & Loretz GmbH	Corn starch	20004426006	2
Caesar & Loretz GmbH	Wheat starch	21000570005	1
Caesar & Loretz GmbH	Wheat starch	21002057001	1
Caesar & Loretz/Geil...	Corn starch	19187802	1
Cealo/Sanacorp	Corn starch	17287302	1
Cealo/Sanacorp	Corn starch	20000573002	1
Cealo	Rice starch	13305103	1
Cealo	Wheat starch	15421507	1
Euro OTC	Wheat starch	104A171122	1
Euro OTC	SyrSpend® SF pH4	18A22-B05-347899	1
Euro OTC	SyrSpend® SF pH4	20F18-F13-379343	1
Euro OTC	Corn starch	64A170123	1
Fagon/Novatis	SyrSpend® SF pH4	20F08-f03	1
Fagron	SyrSpend® SF Alka		2
Fagron	SyrSpend® SF pH4	11111346	1
Fagron	Rice starch	12L19-N06	1
Fagron	Corn starch	14011627	1
Fagron	Rice starch	14F18-B04-301616	1
Fagron	SyrSpend® SF Alka	14I22-B40-311723	1
Fagron	SyrSpend® SF Alka	14J22-B40-311723	2
Fagron	Corn starch	15310902	1
Fagron	SyrSpend® SF pH4	15A26-B04-305667	1
Fagron	SyrSpend® SF Alka	15K03-B01-525173	1
Fagron	SyrSpend® SF pH4	16/10-B03	1
Fagron	SyrSpend® SF pH4	16710-B03	1
Fagron	SyrSpend® SF Alka	16B03-B07-525234	1
Fagron	SyrSpend® SF pH4	16J10_B03_330757	1
Fagron	SyrSpend® SF pH4	16J10B03	1
Fagron	SyrSpend® SF pH4	16J10-B03	3
Fagron	SyrSpend® SF pH4	16j10-b03-330757	1
Fagron	SyrSpend® SF pH4	16J10B03330757	1
Fagron	SyrSpend® SF pH4	16J10-B03-330757	8
Fagron	Corn starch	17287302	1
Fagron	SyrSpend® SF Alka	17D11-804-332593	1
Fagron	SyrSpend® SF Alka	17D11-B04	2
Fagron	SyrSpend® SF Alka	17D11-B04-332593	7
Fagron	SyrSpend® SF Alka	17D11-bo4-332593	1
Fagron	SyrSpend® SF Alka	17D29-B11	1
Fagron	SyrSpend® SF Alka	17F14802-335945	1
Fagron	SyrSpend® SF Alka	17F14B02-335945	1
Fagron	SyrSpend® SF Alka	17F14-B02-335945	5
Fagron	SyrSpend® SF Alka	17F14-B05	1
Fagron	SyrSpend® SF Alka	17F14-B05-525556	2
Fagron	SyrSpend® SF pH4	18/16-B01-357703	1
Fagron	SyrSpend® SF Alka	18/25-B15-357803	1
Fagron	SyrSpend® SF Alka	18125-B15-357803	1
Fagron	SyrSpend® SF Alka	181C13-B11-350851	1
Fagron	SyrSpend® SF Alka	18821-808-147192	1
Fagron	SyrSpend® SF Alka	18821-b08-347192	1
Fagron	SyrSpend® SF Alka	18821-B08-347192	5
Fagron	SyrSpend® SF pH4	18A22_B04_346147	1
Fagron	SyrSpend® SF pH4	18A22-B05	2
Fagron	SyrSpend® SF pH4	18A22-B05-346147	6
Fagron	SyrSpend® SF pH4	18A22-B05-347899	5
Fagron	SyrSpend® SF Alka	18A26-B05	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	SyrSpend® SF Alka	18a26b05346410	1
Fagron	SyrSpend® SF Alka	18A26-B05-346410	4
Fagron	SyrSpend® SF Alka	18A26-Bo5-346410	1
Fagron	SyrSpend® SF Alka	18B21-B08	2
Fagron	SyrSpend® SF Alka	18B21-B08-347192	3
Fagron	SyrSpend® SF Alka	18C13_B11_350851	1
Fagron	SyrSpend® SF Alka	18C13-B11	5
Fagron	SyrSpend® SF Alka	18C13-B11-350851	8
Fagron	SyrSpend® SF Alka	18C-B11-350851	1
Fagron	SyrSpend® SF Alka	18H01-812353473	1
Fagron	SyrSpend® SF Alka	18H01-b12	1
Fagron	SyrSpend® SF Alka	18H01-B12	7
Fagron	SyrSpend® SF Alka	18h01b12353473	1
Fagron	SyrSpend® SF Alka	18H01-B12353473	1
Fagron	SyrSpend® SF Alka	18H01-B12-353473	24
Fagron	SyrSpend® SF Alka	18H13-B12-353473	1
Fagron	SyrSpend® SF pH4	18H30_B02_355226	2
Fagron	SyrSpend® SF pH4	18H30-355226	1
Fagron	SyrSpend® SF pH4	18H30-B02	8
Fagron	SyrSpend® SF pH4	18H30B02355226	1
Fagron	SyrSpend® SF pH4	18H30-B02-355226	9
Fagron	SyrSpend® SF Alka	18I25-B15-357803	1
Fagron	SyrSpend® SF pH4	18J16_B01_357703	1
Fagron	SyrSpend® SF pH4	18J16-B01	2
Fagron	SyrSpend® SF pH4	18J16B01357703	1
Fagron	SyrSpend® SF pH4	18J16-B01-357703	12
Fagron	SyrSpend® SF Alka	18J21B113659901	1
Fagron	SyrSpend® SF Alka	18j25-B15	1
Fagron	SyrSpend® SF Alka	18J25B15	1
Fagron	SyrSpend® SF Alka	18J25-B15	6
Fagron	SyrSpend® SF Alka	18j25b15357803	1
Fagron	SyrSpend® SF Alka	18J25-B15357803	1
Fagron	SyrSpend® SF Alka	18J25-B15-357803	21
Fagron	SyrSpend® SF Alka	18L21-B11	11
Fagron	SyrSpend® SF Alka	18l21-b11-359901	2
Fagron	SyrSpend® SF Alka	18L21B11359901	1
Fagron	SyrSpend® SF Alka	18L21-B11-359901	16
Fagron	SyrSpend® SF Alka	18L21-B113659901	1
Fagron	SyrSpend® SF Alka	18L25-B15-357803	1
Fagron	SyrSpend® SF pH4	19/10-F09-367004	1
Fagron	SyrSpend® SF Alka	19029-B07-362182	1
Fagron	SyrSpend® SF pH4	19A14-B07	3
Fagron	SyrSpend® SF pH4	19A14-B07_362431	1
Fagron	SyrSpend® SF pH4	19A14-B07-362431	5
Fagron	SyrSpend® SF Alka	19D29-807	1
Fagron	SyrSpend® SF Alka	19D29807362182	1
Fagron	SyrSpend® SF Alka	19D29B07	1
Fagron	SyrSpend® SF Alka	19D29-B07	1
Fagron	SyrSpend® SF Alka	19d29b07362182	1
Fagron	SyrSpend® SF Alka	19D29-B07-362182	18
Fagron	SyrSpend® SF Alka	19D29-B11-363786	5
Fagron	SyrSpend® SF Alka	19D29-Bo7-362182	1
Fagron	SyrSpend® SF Alka	19F06-B002	1
Fagron	SyrSpend® SF Alka	19F06-B02	7
Fagron	SyrSpend® SF Alka	19F06-B02_363789	1
Fagron	SyrSpend® SF Alka	19F06-b02-363789	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	SyrSpend® SF Alka	19F06-B02-363789	29
Fagron	SyrSpend® SF Alka	19F12	1
Fagron	SyrSpend® SF Alka	19F12-804-364057	1
Fagron	SyrSpend® SF Alka	19F12-B04	6
Fagron	SyrSpend® SF Alka	19-F12-B04	1
Fagron	SyrSpend® SF Alka	19F12-B04-364057	13
Fagron	SyrSpend® SF Alka	19F12-B04-36-4057	1
Fagron	SyrSpend® SF Alka	19F12-B07	2
Fagron	SyrSpend® SF Alka	19F12-B07-526149	8
Fagron	SyrSpend® SF Alka	19F12-BO4-364057	3
Fagron	SyrSpend® SF pH4	19J10-F08	8
Fagron	SyrSpend® SF pH4	19J10-F08-3669903	1
Fagron	SyrSpend® SF pH4	19j10-F08-366992	1
Fagron	SyrSpend® SF pH4	19J10-F08-366992	2
Fagron	SyrSpend® SF pH4	19J10-f08366993	1
Fagron	SyrSpend® SF pH4	19J10-F08-366993	7
Fagron	SyrSpend® SF pH4	19j10F09	1
Fagron	SyrSpend® SF pH4	19J10-F09	5
Fagron	SyrSpend® SF pH4	19j10-f09-364007	1
Fagron	SyrSpend® SF pH4	19J10-F09-366992	1
Fagron	SyrSpend® SF pH4	19j10-f09-367004	2
Fagron	SyrSpend® SF pH4	19j10-F09-367004	1
Fagron	SyrSpend® SF pH4	19J10-F09-367004	6
Fagron	SyrSpend® SF pH4	19J10-FO8-366992	1
Fagron	SyrSpend® SF Alka	19K007-F04	1
Fagron	SyrSpend® SF Alka	19K07-F04	4
Fagron	SyrSpend® SF Alka	19K07F04367548	1
Fagron	SyrSpend® SF Alka	19K07-F04-367548	5
Fagron	SyrSpend® SF Alka	19k07fo4	1
Fagron	SyrSpend® SF Alka	19K07-FO4-367548	6
Fagron	SyrSpend® SF Alka	19Ko7-F04-367548	1
Fagron	SyrSpend® SF pH4	19L05-F10	5
Fagron	SyrSpend® SF pH4	19L05-F10-3688704	1
Fagron	SyrSpend® SF pH4	19L05-f10-368874	1
Fagron	SyrSpend® SF pH4	19L05-F10-368874	13
Fagron	SyrSpend® SF pH4	19L05-F1O-368874	1
Fagron	SyrSpend® SF pH4	19LO5-F10-368874	1
Fagron	SyrSpend® SF pH4	1BL21-B11	1
Fagron	SyrSpend® SF Alka	20817-F03	1
Fagron	SyrSpend® SF Alka	20818F03	1
Fagron	SyrSpend® SF Alka	20818-F03-369574	3
Fagron	SyrSpend® SF Alka	20825f0625F06	1
Fagron	SyrSpend® SF Alka	20825-F06-369913	3
Fagron	SyrSpend® SF Alka	20825-F07	1
Fagron	SyrSpend® SF Alka	20825-F07-3669914	2
Fagron	SyrSpend® SF Alka	20825-F07369914	2
Fagron	SyrSpend® SF Alka	20825-F07-369914	2
Fagron	SyrSpend® SF Alka	20825-O6-3669913	1
Fagron	SyrSpend® SF Alka	2085-F06	1
Fagron	SyrSpend® SF pH4	20A09-F03	11
Fagron	SyrSpend® SF pH4	20A09-F03-369540	7
Fagron	SyrSpend® SF pH4	20A09-F03-3695400	1
Fagron	SyrSpend® SF Alka	20B18-F03	3
Fagron	SyrSpend® SF Alka	20B18-F03-369574	10
Fagron	SyrSpend® SF Alka	20B25-F06	4
Fagron	SyrSpend® SF Alka	20B25-F06_369913	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	SyrSpend® SF Alka	20B25-F06-369913	29
Fagron	SyrSpend® SF Alka	20B25-F07	8
Fagron	SyrSpend® SF Alka	20B25-F07-369914	9
Fagron	SyrSpend® SF Alka	20B25-FO7-369914	1
Fagron	SyrSpend® SF Alka	20B818-F03-369574	2
Fagron	SyrSpend® SF pH4	20c24-F02	1
Fagron	SyrSpend® SF pH4	20C24-F02	8
Fagron	SyrSpend® SF pH4	20c24-f02-372398	1
Fagron	SyrSpend® SF pH4	20c24-F02-372398	1
Fagron	SyrSpend® SF pH4	20C24-F02-372398	17
Fagron	SyrSpend® SF pH4	20C24-F09	1
Fagron	SyrSpend® SF pH4	20C24-FO2	2
Fagron	SyrSpend® SF Alka	20D15-F08	1
Fagron	SyrSpend® SF Alka	20D15-F08-371028	2
Fagron	SyrSpend® SF Alka	20D16-F01	1
Fagron	SyrSpend® SF Alka	20D16-F06	1
Fagron	SyrSpend® SF pH4	20F08_F03_372517	1
Fagron	SyrSpend® SF pH4	20F08-F03	5
Fagron	SyrSpend® SF pH4	20F08-F03-0000	1
Fagron	SyrSpend® SF pH4	20F08-F03-372517	19
Fagron	SyrSpend® SF pH4	20F08-F04-372518	1
Fagron	SyrSpend® SF pH4	20F18-F13-379343	22
Fagron	SyrSpend® SF pH4	20F18-F14	2
Fagron	SyrSpend® SF Alka	20F18-F14-379344	11
Fagron	SyrSpend® SF Alka	20G03-F09-526400	1
Fagron	SyrSpend® SF Alka	20G03-F11	3
Fagron	SyrSpend® SF Alka	20G03-F11-374279	20
Fagron	SyrSpend® SF Alka	20G03-F12	2
Fagron	SyrSpend® SF Alka	20G03-F12-374282	6
Fagron	SyrSpend® SF Alka	20Go3-f12-374282	1
Fagron	SyrSpend® SF Alka	21101_F-02	1
Fagron	SyrSpend® SF Alka	21101-F02	1
Fagron	SyrSpend® SF Alka	21101-F02-380031	4
Fagron	SyrSpend® SF pH4	211021-01	1
Fagron	SyrSpend® SF Alka	21826-F08	1
Fagron	SyrSpend® SF Alka	21826-F08-379141	2
Fagron	SyrSpend® SF Alka	21926-F07-378133	1
Fagron	SyrSpend® SF Alka	21A21-376829	3
Fagron	SyrSpend® SF Alka	21A21-F01	5
Fagron	SyrSpend® SF Alka	21A21-F01-376829	18
Fagron	SyrSpend® SF Alka	21A21-FO1	1
Fagron	SyrSpend® SF Alka	21B26-F06	2
Fagron	SyrSpend® SF Alka	21B26-F07-378133	9
Fagron	SyrSpend® SF Alka	21B26-F08	2
Fagron	SyrSpend® SF Alka	21B26-F08-379141	10
Fagron	SyrSpend® SF Alka	21B26-FO6	1
Fagron	SyrSpend® SF Alka	21B26-FO7378133	1
Fagron	SyrSpend® SF Alka	21F08-F03	3
Fagron	SyrSpend® SF Alka	21F08F03378828	1
Fagron	SyrSpend® SF Alka	21F08-F03-378828	20
Fagron	SyrSpend® SF Alka	21F08-F04	1
Fagron	SyrSpend® SF Alka	21F08-F04-378832	5
Fagron	SyrSpend® SF Alka	21F24F01379228	1
Fagron	SyrSpend® SF Alka	21F24-F01-379228	17
Fagron	SyrSpend® SF Alka	21F24-F01-37928	1
Fagron	SyrSpend® SF Alka	21F24-F03-379228	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	SyrSpend® SF Alka	21F24-F03526598	1
Fagron	SyrSpend® SF Alka	21F24-F03-526598	3
Fagron	SyrSpend® SF Alka	21F24-F04	2
Fagron	SyrSpend® SF Alka	21F24-F04-379672	4
Fagron	SyrSpend® SF Alka	21F24-F01	1
Fagron	SyrSpend® SF Alka	21F08-F03-378828	1
Fagron	SyrSpend® SF Alka	21H16-F06	1
Fagron	SyrSpend® SF Alka	21H16-F06-0000	1
Fagron	SyrSpend® SF Alka	21H16F06379894	1
Fagron	SyrSpend® SF Alka	21H16-F06-379894	27
Fagron	SyrSpend® SF Alka	21H16-F06	1
Fagron	SyrSpend® SF pH4	21H20-F02-380674	9
Fagron	SyrSpend® SF Alka	21I01-F02	1
Fagron	SyrSpend® SF Alka	21I01-F02-380031	28
Fagron	SyrSpend® SF pH4	21K22-F06	1
Fagron	SyrSpend® SF Alka	21l01-F02-380031	1
Fagron	SyrSpend® SF Alka	21L07-F04-381033	2
Fagron	SyrSpend® SF Alka	21L07-F05	5
Fagron	SyrSpend® SF Alka	21L07F05381032	1
Fagron	SyrSpend® SF Alka	21L07-F05-381032	42
Fagron	SyrSpend® SF Alka	21L-07-F05-381032	1
Fagron	SyrSpend® SF pH4	22007-F04	1
Fagron	SyrSpend® SF pH4	22109-F02	1
Fagron	SyrSpend® SF pH4	22109-F03-383490	1
Fagron	SyrSpend® SF Alka	22804-F06	1
Fagron	SyrSpend® SF Alka	22804-F06-381564	1
Fagron	SyrSpend® SF Alka	22A12F20381408	1
Fagron	SyrSpend® SF Alka	22A12-F20-381408	5
Fagron	SyrSpend® SF Alka	22A12-F21	1
Fagron	SyrSpend® SF Alka	22A12F21526828	1
Fagron	SyrSpend® SF Alka	22A12-F21-526828	3
Fagron	SyrSpend® SF Alka	22A12-F22-382195	11
Fagron	SyrSpend® SF Alka	22A12-F24-382104	5
Fagron	SyrSpend® SF Alka	22B04-F04-381555	2
Fagron	SyrSpend® SF Alka	22B04F05-3819009	1
Fagron	SyrSpend® SF Alka	22B04-F05-381909	2
Fagron	SyrSpend® SF Alka	22B04-F05-381975	1
Fagron	SyrSpend® SF Alka	22B04-F06	2
Fagron	SyrSpend® SF Alka	22B04F06-381564	1
Fagron	SyrSpend® SF Alka	22B04-F06-381564	12
Fagron	SyrSpend® SF Alka	22B04-F07-381936	2
Fagron	SyrSpend® SF pH4	22B04-F02381139	1
Fagron	SyrSpend® SF Alka	22B04-F06-381564	1
Fagron	SyrSpend® SF pH4	22C07-F03	2
Fagron	SyrSpend® SF pH4	22C07-F03-382305	6
Fagron	SyrSpend® SF pH4	22C07-F04	1
Fagron	SyrSpend® SF pH4	22C07-F04-0000	1
Fagron	SyrSpend® SF pH4	22C07F04382813	1
Fagron	SyrSpend® SF pH4	22C07-F04-382813	8
Fagron	SyrSpend® SF pH4	22G07-H08	1
Fagron	SyrSpend® SF pH4	22I09-F01-383384	3
Fagron	SyrSpend® SF pH4	22I09-F02-383489	8
Fagron	SyrSpend® SF Alka	22J04-F02-383639	7
Fagron	SyrSpend® SF Alka	22J04-F0-2383639	1
Fagron	SyrSpend® SF Alka	22J04-F06-383652	10
Fagron	SyrSpend® SF Alka	22J31-F01-526993	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	SyrSpend® SF Alka	22J4-F06-383652	1
Fagron	SyrSpend® SF pH4	22J04-F06-383652	1
Fagron	SyrSpend® SF pH4	22K01-H01	1
Fagron	SyrSpend® SF pH4	22K08F02-383826	1
Fagron	SyrSpend® SF pH4	22K08-F02-383826	6
Fagron	SyrSpend® SF pH4	22109-F01-383384	1
Fagron	SyrSpend® SF pH4	22109-F03-383490	1
Fagron	SyrSpend® SF pH4	22L20-F03-384076	1
Fagron	SyrSpend® SF pH4	23A03-F10-384538	1
Fagron	SyrSpend® SF pH4 neo (Mai…	23J11-H01-00941	1
Fagron	SyrSpend® SF pH4 neo (Mai…	24B28-H08-00941	1
Fagron	SyrSpend® SF Alka	2IL07-F05-381032	1
Fagron	SyrSpend® SF Alka	20B18F03369574	1
Fagron	SyrSpend® SF Alka	318828	1
Fagron	SyrSpend® SF Alka	379672	1
Fagron	SyrSpend® SF Alka	6369913	1
Fagron	SyrSpend® SF Alka	720026-0000	2
Fagron	SyrSpend® SF Alka	7-378133	1
Fagron	SyrSpend® SF Alka	802-3637809	1
Fagron	SyrSpend® SF Alka	B02-3637809	4
Fagron	SyrSpend® SF Alka	B04-3640507	1
Fagron	SyrSpend® SF Alka	B07-5261409	3
Fagron	SyrSpend® SF Alka	F01-3768209	2
Fagron	SyrSpend® SF Alka	F01-376829	2
Fagron	SyrSpend® SF pH4	F02-3723908	4
Fagron	SyrSpend® SF Alka	F02-3800301	1
Fagron	SyrSpend® SF pH4	F02-3834809	3
Fagron	SyrSpend® SF pH4	F03-3695400	1
Fagron	SyrSpend® SF Alka	F03-3695704	2
Fagron	SyrSpend® SF pH4	F03-3725107	1
Fagron	SyrSpend® SF Alka	F03-3788208	1
Fagron	SyrSpend® SF Alka	F0538103002	1
Fagron	SyrSpend® SF Alka	F06-3699103	3
Fagron	SyrSpend® SF Alka	F06-369913	1
Fagron	SyrSpend® SF Alka	F07-3699104	3
Fagron	SyrSpend® SF Alka	F07-3781303	1
Fagron	SyrSpend® SF Alka	F07-3788300	2
Fagron	SyrSpend® SF pH4	F08-3669902	1
Fagron	SyrSpend® SF pH4	F08-3669903	2
Fagron	SyrSpend® SF Alka	F08-3791401	2
Fagron	SyrSpend® SF pH4	F09-3670004	1
Fagron	SyrSpend® SF pH4	F10-3688704	2
Fagron	SyrSpend® SF Alka	F1137427009	3
Fagron	SyrSpend® SF Alka	F11-3742709	3
Fagron	SyrSpend® SF Alka	F12-3748002	1
Fagron	SyrSpend® SF pH4	FO3-3725107	1
Fagron	SyrSpend® SF Alka	FO4-3815505	1
Fagron	SyrSpend® SF Alka	FO6-3798904	1
Fargon / AHD	SyrSpend® SF Alka	20G03-F09-526400	1
Fargon/AHD	SyrSpend® SF Alka	18C13-B11	1
Fargon/Phönix	SyrSpend® SF Alka	20B25-F06-369913	2
Fargon	SyrSpend® SF Alka	19F12-BO4-364057	1
Fargon	SyrSpend® SF Alka	21B26F07378133	1
Fiebig 16.01.13 ek: 4,18EUR	Wheat starch	11350911	1
Fiebig	Wheat starch	104A201028-01	1
Fiebig	SyrSpend® SF pH4	20F08-F03	1
Fiebig	Corn starch	64A170123	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fischar/Gehe	SyrSpend® SF Alka	18L21-B11-359901	1
Fragon/ Noweda	SyrSpend® SF Alka	19F12-B04-364057	2
Fragron / Gehe	SyrSpend® SF Alka	20G03-F11-374279	1
Fresenius	Wheat starch	13305103	1
Gehe	Wheat starch	1028-01	1
Gehe	Corn starch	16138505	1
Gehe	Corn starch	17287302	1
Gehe	Corn starch	17287305	1
Gehe	Corn starch	18274802	2
Gehe	SyrSpend® SF Alka	18A26-B05-346410	1
Gehe	SyrSpend® SF Alka	18H01-B12-353473	10
Gehe	SyrSpend® SF pH4	18J16-B01-357703	3
Gehe	SyrSpend® SF Alka	18L21-B11	1
Gehe	Corn starch	19187802	1
Gehe	SyrSpend® SF pH4	19A14-B07-362431	1
Gehe	Corn starch	64A130304	1
Gutenberg-Apotheke	Rice starch	12360216	1
Kehr	Wheat starch	104A160512	1
Kehr	SyrSpend® SF pH4	22L20-F03-384076	1
Kehr	SyrSpend® SF pH4	23E22-F01-384947	1
Klemk	Wheat starch	104A160512	1
Klenk	Wheat starch	101A201028-01	1
Klenk	Wheat starch	1028-01	1
Klenk	Wheat starch	104A101116	1
Klenk	Rice starch	104A120621	5
Klenk	Rice starch	104A130304	8
Klenk	Wheat starch	104a141114	1
Klenk	Rice starch	104A141114	9
Klenk	Wheat starch	104a160512	1
Klenk	Wheat starch	104A160512	8
Klenk	Wheat starch	104a171122	1
Klenk	Wheat starch	104A171122	12
Klenk	Wheat starch	104A19100101	1
Klenk	Wheat starch	104A191001-01	3
Klenk	Wheat starch	104A200107-01	2
Klenk	Wheat starch	104A201028-01	4
Klenk	Wheat starch	104A210720-01	1
Klenk	Wheat starch	104A221027-01	2
Klenk	Wheat starch	10720-01	1
Klenk	Corn starch	10816-01	1
Klenk	Wheat starch	10A160512	1
Klenk	Wheat starch	10A201028-01	1
Klenk	Wheat starch	191001-001	1
Klenk	Corn starch	200427-001	2
Klenk	Rice starch	200921-002	1
Klenk	Corn starch	220328A	1
Klenk	Corn starch	4263535	1
Klenk	Corn starch	427-01	1
Klenk	Rice starch	64A080218	5
Klenk	Rice starch	64a130304	1
Klenk	Rice starch	64A130304	18
Klenk	Corn starch	64A170123	31
Klenk	Corn starch	64A181203	15
Klenk	Corn starch	64A20042701	2
Klenk	Corn starch	64A200427-01	17
Klenk	Corn starch	64-A-200427-01	1
Klenk	Corn starch	64A21081601	1
Klenk	Corn starch	64A210816-01	2
Klenk	Corn starch	6A181203	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Potato starch	80919-01	1
Klenk	Rice starch	84A130304	1
Klenk	Rice starch	84A141114	4
Klenk	Rice starch	84A180522	2
Klenk	Wheat starch	91001-01	1
Klenk	Rice starch	94A100122	1
Klenk	Potato starch	94A110512	1
Klenk	Rice starch	94A130304	5
Klenk	Potato starch	94a170123	1
Klenk	Potato starch	94A170123	4
Klenk	Potato starch	94A180919	1
Klenk	Potato starch	94A180919-01	3
Klosterring	Wheat starch	15421507	1
Koisser	Rice starch	WE07032013	1
Krieger	SyrSpend® SF Alka	22B04-F06-381564	1
Nachprüfung	Wheat starch	3082019-1	1
Nachprüfung	Rice starch	3709E01116	1
Nachprüfung	Corn starch	AP200525-12	1
Noweda/Hedinger	SyrSpend® SF pH4	18J16-B01-357703	1
Noweda	Wheat starch	104A221027-01	1
Noweda	Rice starch	14011621	1
Noweda	Rice starch	14023203	1
noweda	SyrSpend® SF pH4	15I22-B02-52176	1
Noweda	SyrSpend® SF Alka	18L21-B11-359901	1
Noweda	Corn starch	20004426006	1
Noweda	Corn starch	20004426018	1
Noweda	Rice starch	20004428009	1
Noweda	SyrSpend® SF Alka	20B25-F07	1
Noweda	SyrSpend® SF pH4	2209-F03-383490	1
Noweda	SyrSpend® SF Alka	22A12-F22-382195	1
Noweda	SyrSpend® SF pH4	22I09-F02-383489	1
Noweda	SyrSpend® SF pH4	22I09-F03-383490	1
Noweda	SyrSpend® SF Alka	22J04-F02-383639	1
Noweda	SyrSpend® SF Alka	22J31-F01-526993	1
Noweda	SyrSpend® SF Alka	22J04-F06-383652	1
Phoenix	SyrSpend® SF pH4	18H30-B02-355226	1
Phoenix	SyrSpend® SF pH4	18J25-B15-357803	1
Phoenix	SyrSpend® SF Alka	18L21-B11-359901	6
Phoenix	SyrSpend® SF Alka	19D29-B07-362182	4
Phoenix	SyrSpend® SF Alka	19D29-B11-363786	3
Phoenix	SyrSpend® SF Alka	F03-3788208	1
Phönix/Fagon	SyrSpend® SF Alka	17D11-B04-332593	1
Phönix	Wheat starch	104A191001-01	1
PHönix	Wheat starch	104A210720-01	1
PHÖNIX	Wheat starch	16162905	1
Phönix	SyrSpend® SF pH4	16J10-B03-330757	3
Phönix	SyrSpend® SF Alka	18B13-B11-350851	1
Phönix	SyrSpend® SF pH4	18H30-B02-355226	8
Phönix	SyrSpend® SF Alka	19F12-B04-364057	1
Phönix	SyrSpend® SF Alka	21F08-F03378828	1
Phönix	SyrSpend® SF Alka	21L07-F05	3
Phönix	SyrSpend® SF Alka	22B04-F04-381555	8
phönix	Rice starch	84a141114	1
Phönix	Rice starch	84A141114	2
Sanacorp	Corn starch	18274808	1
Sanacorp	SyrSpend® SF Alka	21F08-F03-378828	1
Sanacorp	SyrSpend® SF Alka	21F08-F03-378828210166	1
Sanacorp	SyrSpend® SF Alka	22804-F07	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	SyrSpend® SF Alka	22J04-F11-383746	2
Sanacorp	SyrSpend® SF Alka	23A18-F07-384725	2
Sanacorp	SyrSpend® SF pH4	23E22-F02-384949	1
Sanacorp	SyrSpend® SF pH4 neo (Mai…	24H06-H07-00941	1
Sanacorp	Corn starch	64A181203	1
Sanacorp	Rice starch	84A141114	1
sanacorp	Rice starch	94A130304	1
Spinnrad GmbH	Corn starch	519408192	1
VDL;03.03.15;3,04EUR	Rice starch	14011627	1
VDL;3,03EUR;11.06.15	Rice starch	14011630	1

- 234 230 spectra from 1515 *Apo-Ident* customers from a total of 48 721 batches from a further 715 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Starch* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Starch* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	1860	0	151 102
Type B	0	1550	0	200 520
Type C	0	1836	1	234 200

The substance/substance group *Starch* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.6774 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.6129 %)
Type C	100.0000 % (> 99.9005 %)	99.9456 % (> 99.7823 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20790	22450	8.42	55.22
20996	20996	0.00	69.99
21447	21447	0.00	52.38
21827	22450	5.88	58.62
21965	22449	6.69	73.62
21973	22450	7.82	58.65
22246	22450	11.25	56.17
22449	22449	0.00	69.11
22450	22450	0.00	60.73
22496	22496	0.00	40.22
22497	22496	2.10	40.49
22585	25767	8.40	52.41
22719	22719	0.00	32.16
23219	23220	7.25	38.42
23220	23220	0.00	45.49
23448	24112	16.67	52.30
23449	24112	16.23	51.72
23510	21447	12.60	59.20
23750	23750	0.00	54.00
23923	22449	7.15	71.27
24112	24112	0.00	61.76
24290	24112	7.29	60.22
24361	24361	0.00	59.51
25080	25080	0.00	29.89
25363	24112	17.20	48.27
25369	22496	9.96	38.61
25382	22449	9.77	68.40
25383	22450	9.33	48.80
25534	25534	0.00	34.02
25755	25755	0.00	41.97
25767	25767	0.00	50.42
26568	22496	15.58	35.86
26613	22496	5.72	39.73
26677	22496	9.73	37.72
27029	24112	24.85	46.06
27030	22496	18.08	38.51
27056	22496	14.41	44.79
27107	27107	0.00	54.88
27180	22496	11.68	38.34
27192	22496	14.61	43.53
27321	27321	0.00	71.57
27324	27324	0.00	55.98

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Stearic acid 50**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20869-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Stearic acid 50; Acidum stearicum

Special notes

When selecting the *Stearic acid 50* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Stearic acid 50	6	4	36

Second-stage model

For differentiation of the substance/substance group *Stearic acid 50* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Stearic acid 50* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Hard fat	93.84	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Stearic acid 50* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Stearic acid 50*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Stearic acid 50	12241910	20869	40	AR-15-FG-007284-01
Caelo	Stearic acid 50	14359310	21793	60	20150126
Caelo	Stearic acid 50	14359310	21928	60	AR-16-FG-004044-01
Caelo	Stearic acid 50	14359314	22274	60	20150126
Caelo	Stearic acid 50	170810	23294	40	20170426*
Caelo	Stearic acid 50	170810	23667	40	20170426*
Caelo	Stearic acid 50	192910	25066	40	20191128*
Caelo	Stearic acid 50	22000750	26125	30	20220429*
Caelo	Stearic acid 50	22000750	26125SI	20	20220429*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 390 spectra of 9 reference samples from the substance/substance group *Stearic acid 50*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 572 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 5 reference samples from the substance/substance group *Stearic acid 50*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Stearic acid 50	163469	23032	40
Caelo	Stearic acid 50	180809	24036	40
Caelo	Stearic acid 50	20003933010	25731	50
Caelo	Stearic acid 50	23001610	26833	40
Caelo	Stearic acid 50	23001610	26833SI	20

- 201 894 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 88 spectra from 42 *Apo-Ident* customers from 39 batches from the substance/substance group *Stearic acid 50*.

- Among them are spectra of independent samples from 36 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Stearic acid 50	23001610002	1
Caelo	Stearic acid 50	11103706	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Stearic acid 50	11308505	1
Caelo	Stearic acid 50	11308514	1
Caelo	Stearic acid 50	12241911	2
Caelo	Stearic acid 50	12241914	1
Caelo	Stearic acid 50	12241915	2
Caelo	Stearic acid 50	12241930	3
Caelo	Stearic acid 50	14359314	4
Caelo	Stearic acid 50	1609611	1
Caelo	Stearic acid 50	16096301	2
Caelo	Stearic acid 50	16096311	1
Caelo	Stearic acid 50	1617081006	1
Caelo	Stearic acid 50	17081003	1
Caelo	Stearic acid 50	17081006	5
Caelo	Stearic acid 50	1808013	1
Caelo	Stearic acid 50	18080901	4
Caelo	Stearic acid 50	18080913	4
Caelo	Stearic acid 50	18238002	1
Caelo	Stearic acid 50	18238004	5
Caelo	Stearic acid 50	18238006	2
Caelo	Stearic acid 50	18238010	4
Caelo	Stearic acid 50	192910002	1
Caelo	Stearic acid 50	192910005	2
Caelo	Stearic acid 50	192910010	1
Caelo	Stearic acid 50	192910012	1
Caelo	Stearic acid 50	2000393001	1
Caelo	Stearic acid 50	20003933002	1
Caelo	Stearic acid 50	21003445001	1
Caelo	Stearic acid 50	21003445002	1
Caelo	Stearic acid 50	22000750004	4
Caelo	Stearic acid 50	23933002	1
Caesar & Loretz GmbH…	Stearic acid 50	18238010	1
Caesar & Loretz GmbH…	Stearic acid 50	20003933002	1
Caesar & Loretz GmbH…	Stearic acid 50	18238006	1
Caesar & Loretz GmbH…	Stearic acid 50	192910	1
Caesar & Loretz GmbH…	Stearic acid 50	18238006	1
Caesar & Loretz GmbH	Stearic acid 50	18238010	1
Caesar & Loretz GmbH	Stearic acid 50	192910005	5
Caesar & Loretz GmbH	Stearic acid 50	20003933001	3
Caesar & Loretz GmbH	Stearic acid 50	20003933010	1
Caesar & Loretz GmbH	Stearic acid 50	21003445002	1
Caesar & Loretz	Stearic acid 50	14359310	1
Caesar&Loretz GmbH/Anzag	Stearic acid 50	11308505	1
Caleo	Stearic acid 50	16096301	1
GEHE	Stearic acid 50	18238006	1
Jenne	Stearic acid 50	18080901	1
Kehr	Stearic acid 50	16346902	1
Phoenix	Stearic acid 50	12241915	1
Phönix	Stearic acid 50	1224915	1
Phönix	Stearic acid 50	18080901	1
ROHA	Stearic acid 50	130240	1

- 235 979 spectra from 1515 *Apo-Ident* customers from a total of 49 219 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Stearic acid 50* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Stearic acid 50* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	390	0	152 572
Type B	0	190	0	201 894
Type C	0	86	2	235 979

The substance/substance group *Stearic acid 50* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4615 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9007 %)	97.7273 % (> 94.3182 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20869	20869	0.00	127.02
21793	21928	7.15	125.15
21928	21928	0.00	130.91
22274	25066	6.93	122.40
23294	23294	0.00	122.97
23667	23667	0.00	121.78
25066	25066	0.00	122.93
26125	26125	0.00	131.50

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sucrose**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20372-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sucrose; Saccharum

Special notes

When selecting the *Sucrose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sucrose	13	8	696

Second-stage model

For differentiation of the substance/substance group *Sucrose* the following second-stage model is used:

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sucrose* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	57.03	–
⋮	⋮	⋮
Sodium citrate	>50	76.51
Heparin sodium	>50	122.97
Capsaicin	>50	255.90
Amifampridine	>50	421.29
Quinine hydrochloride dihydrate	>50	459.42
Oxybutynin hydrochloride	>50	515.33
Levocarnitine	>50	554.22
Prednicarbate	>50	618.68
Pyridoxal-5-phosphate	>50	661.74
Ciprofloxacin hydrochloride	>50	836.42
Methoxsalen	>50	910.90
Triclosan	>50	917.45
Alfatradiol	>50	967.42
Tetracaine	>50	1084.88
Cyproterone acetate	>50	1479.83
Norethisterone acetate	>50	1574.56
Amitriptyline hydrochloride	>50	2918.29
Valine	>50	3858.21

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sucrose* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sucrose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sucrose	13352909	21484	40	1410501
Caelo	Sucrose	14340003	21736	60	20141114
Caelo	Sucrose	161999	22615	40	20160714*
Caelo	Sucrose	162060	22643	40	20160808*
Caelo	Sucrose	163286	23057	40	20161219*
Caelo	Sucrose	163081	23058	40	20161115*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sucrose	171066	23297	40	20170511*
Caelo	Sucrose	172133	23666	40	20170817*
Caelo	Sucrose	173247	23833	40	20180117*
Caelo	Sucrose	181582	24217	40	20180605*
Caelo	Sucrose	21000656	25651	40	20210406*
Caelo	Sucrose	22002704	26630	40	20220909*
Caelo	Sucrose	22002704	26630SI	20	20220909*
Caelo	Sucrose	23000893	26723	40	20230601*
Caelo	Sucrose	23000893	26723SI	20	20230601*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 580 spectra of 15 reference samples from the substance/substance group *Sucrose*. These samples are listed above in the *calibration samples* section. The reference samples come from 13 different batches.

- 152 382 spectra from a total of 2829 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 340 spectra of 9 reference samples from the substance/substance group *Sucrose*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sucrose	12146801	20909	40
Caelo	Sucrose	181546	24237	40
Caelo	Sucrose	182574	24353	40
Caelo	Sucrose	182818	24359	40
Caelo	Sucrose	192839	25235	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sucrose	190627	25236	40
Caelo	Sucrose	24000032	27134	40
Caelo	Sucrose	24002338	27447	40
Caelo	Sucrose	24000032	27134SI	20

- 201 744 spectra from a total of 4037 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1771 spectra from 483 *Apo-Ident* customers from 700 batches from the substance/substance group *Sucrose*.
- Among them are spectra of independent samples from 695 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Sucrose	13352908	1
	Sucrose	21003804004	3
	Sucrose	21003804007	1
	Sucrose	21003804012	9
	Sucrose	22002704004	10
	Sucrose	22002704005	2
	Sucrose	2202704004	1
	Sucrose	222704004	1
	Sucrose	23000893002	6
	Sucrose	23003269004	3
AHD	Sucrose	15182805	1
AHD	Sucrose	18154602	1
AHD	Sucrose	18154603	2
Audor Pharma	Sucrose	16206102	1
Bombastus	Sucrose	15156008	1
Cael	Sucrose	15182804	3
Caelo	Sucrose		1
Caelo	Sucrose	1(192839004)	1
Caelo	Sucrose	11246306	1
Caelo	Sucrose	11246313	2
Caelo	Sucrose	12107805	1
Caelo	Sucrose	12107806	2
Caelo	Sucrose	12241801	1
Caelo	Sucrose	12241803	2
Caelo	Sucrose	12241804	2
Caelo	Sucrose	12241808	5
Caelo	Sucrose	12241817	2
Caelo	Sucrose	12280309	1
Caelo	Sucrose	130031417	1
Caelo	Sucrose	13031405	3
Caelo	Sucrose	13031406	2
Caelo	Sucrose	13031409	1
Caelo	Sucrose	13031410	2
Caelo	Sucrose	13031414	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sucrose	13031417	2
Caelo	Sucrose	13063907	1
Caelo	Sucrose	13111706	1
Caelo	Sucrose	13352901	2
Caelo	Sucrose	13352902	13
Caelo	Sucrose	13352905	1
Caelo	Sucrose	13352908	1
Caelo	Sucrose	13352909	4
Caelo	Sucrose	13352911	1
Caelo	Sucrose	13352916	3
Caelo	Sucrose	13352920	5
Caelo	Sucrose	1352920	1
Caelo	Sucrose	14197301	4
Caelo	Sucrose	14197302	3
Caelo	Sucrose	14197313	1
Caelo	Sucrose	1430009	1
Caelo	Sucrose	14340003	4
Caelo	Sucrose	14340004	5
Caelo	Sucrose	14340005	1
Caelo	Sucrose	14340006	1
Caelo	Sucrose	14340008	5
Caelo	Sucrose	14340009	4
Caelo	Sucrose	15028801	14
Caelo	Sucrose	15028802	7
Caelo	Sucrose	15156008	1
Caelo	Sucrose	15182804	25
Caelo	Sucrose	15182805	3
Caelo	Sucrose	154460	1
Caelo	Sucrose	15446002	11
Caelo	Sucrose	15446003	7
Caelo	Sucrose	15446007	1
Caelo	Sucrose	160499	1
Caelo	Sucrose	16049902	3
Caelo	Sucrose	16049907	17
Caelo	Sucrose	16051301	1
Caelo	Sucrose	16051304	1
Caelo	Sucrose	16051305	2
Caelo	Sucrose	16166003	1
Caelo	Sucrose	162061	1
Caelo	Sucrose	16206102	13
Caelo	Sucrose	16206103	6
Caelo	Sucrose	1628603	1
Caelo	Sucrose	16305501	1
Caelo	Sucrose	16325605	1
Caelo	Sucrose	16328603	12
Caelo	Sucrose	16328605	22
Caelo	Sucrose	16328606	7
Caelo	Sucrose	16328607	22
Caelo	Sucrose	16351702	1
Caelo	Sucrose	1649902	1
Caelo	Sucrose	17021620306	1
Caelo	Sucrose	17042103	4
Caelo	Sucrose	17106601	1
Caelo	Sucrose	17106603	57
Caelo	Sucrose	17106604	22
Caelo	Sucrose	17247203	1
Caelo	Sucrose	17288702	1
Caelo	Sucrose	17354506	20
Caelo	Sucrose	18024405	41
Caelo	Sucrose	18024407	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sucrose	1802445	1
Caelo	Sucrose	18154602	15
Caelo	Sucrose	18154603	28
Caelo	Sucrose	18257401	16
Caelo	Sucrose	18257402	52
Caelo	Sucrose	18260801	1
Caelo	Sucrose	18281803	4
Caelo	Sucrose	18281804	23
Caelo	Sucrose	18281810	2
Caelo	Sucrose	18329702	29
Caelo	Sucrose	18329703	9
Caelo	Sucrose	19060320648	1
Caelo	Sucrose	19060320649	1
Caelo	Sucrose	19060320650	1
Caelo	Sucrose	190627001	3
Caelo	Sucrose	190627002	23
Caelo	Sucrose	19062701	41
Caelo	Sucrose	19062702	4
Caelo	Sucrose	19132301	2
Caelo	Sucrose	1928339004	1
Caelo	Sucrose	192839001	1
Caelo	Sucrose	192839002	5
Caelo	Sucrose	192839004	33
Caelo	Sucrose	192839006	4
Caelo	Sucrose	192839007	26
Caelo	Sucrose	1928839004	1
Caelo	Sucrose	2(192839007)	1
Caelo	Sucrose	20001028003	1
Caelo	Sucrose	20002000004	1
Caelo	Sucrose	20003141002	1
Caelo	Sucrose	20003432001	1
Caelo	Sucrose	20004028001	3
Caelo	Sucrose	20004028003	22
Caelo	Sucrose	20011401	1
Caelo	Sucrose	20031515	1
Caelo	Sucrose	2100065004	1
Caelo	Sucrose	2100065006	1
Caelo	Sucrose	2100065007	1
Caelo	Sucrose	210006560001	1
Caelo	Sucrose	21000656001	22
Caelo	Sucrose	21000656004	4
Caelo	Sucrose	21000656006	11
Caelo	Sucrose	21000656007	4
Caelo	Sucrose	21000656010	12
Caelo	Sucrose	21003804003	4
Caelo	Sucrose	21003804004	18
Caelo	Sucrose	21003804007	7
Caelo	Sucrose	21003804008	2
Caelo	Sucrose	21003804011	1
Caelo	Sucrose	21003804012	3
Caelo	Sucrose	21003804013	2
Caelo	Sucrose	2100380412	1
Caelo	Sucrose	21003B	1
Caelo	Sucrose	22002704004	1
Caelo	Sucrose	24061502	1
Caelo	Sucrose	27111802	1
Caelo	Sucrose	28041504	1
Caelo	Sucrose	28081308	1
Caelo	Sucrose	29081502	1
Caelo	Sucrose	4028003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sucrose	8024405	1
Caelo	Sucrose	81172478	2
Caelo	Sucrose	8704717	1
Caelo	Sucrose	Caelo14197301	1
Caeol/ Sanacorp	Sucrose	21000656001	1
Caeol/Sanacorp	Sucrose	18154603	1
Caeolo/Gehe	Sucrose	15446002	1
Caeolo/NOWEDA	Sucrose	21003804008	1
Caesar & Loretz GmbH...	Sucrose	16049907	1
Caesar & Loretz GmbH...	Sucrose	192839006	2
Caesar & Loretz GmbH...	Sucrose	21000656007	1
Caesar & Loretz GmbH...	Sucrose	192839006	1
Caesar & Loretz GmbH...	Sucrose	192839007	1
Caesar & Loretz GmbH...	Sucrose	190627002	1
Caesar & Loretz GmbH...	Sucrose	20004028003	1
Caesar & Loretz GmbH...	Sucrose	20004028003	2
Caesar & Loretz GmbH...	Sucrose	21000656010	1
Caesar & Loretz GmbH/G	Sucrose	18257402	1
Caesar & Loretz GmbH/Gehe	Sucrose	192839007	1
Caesar & Loretz GmbH/Gehe	Sucrose	20004028003	1
Caesar & Loretz GmbH/Gehe	Sucrose	21003804004	1
Caesar & Loretz GmbH...	Sucrose	192839006	1
Caesar & Loretz GmbH...	Sucrose	21000656007	1
Caesar & Loretz GmbH...	Sucrose	18281804	2
Caesar & Loretz GmbH...	Sucrose	18329703	1
Caesar & Loretz GmbH...	Sucrose	192839004	1
Caesar & Loretz GmbH...	Sucrose	19062701	3
Caesar & Loretz GmbH...	Sucrose	21000656001	1
Caesar & Loretz GmbH...	Sucrose	21003804012	1
Caesar & Loretz GmbH/Sana	Sucrose	20004028001	1
Caesar & Loretz GmbH...	Sucrose	17354506	1
Caesar & Loretz GmbH...	Sucrose	190627002	1
Caesar & Loretz GmbH...	Sucrose	19062701	1
Caesar & Loretz GmbH...	Sucrose	192839007	1
Caesar & Loretz GmbH...	Sucrose	21000656001	1
Caesar & Loretz GmbH...	Sucrose	21000656006	1
Caesar & Loretz GmbH	Sucrose	16328605	1
Caesar & Loretz GmbH	Sucrose	18154601	1
Caesar & Loretz GmbH	Sucrose	18154603	1
Caesar & Loretz GmbH	Sucrose	18257401	4
Caesar & Loretz GmbH	Sucrose	18257402	7
Caesar & Loretz GmbH	Sucrose	18281803	1
Caesar & Loretz GmbH	Sucrose	18281804	8
Caesar & Loretz GmbH	Sucrose	18329702	10
Caesar & Loretz GmbH	Sucrose	18329703	2
Caesar & Loretz GmbH	Sucrose	190627001	2
Caesar & Loretz GmbH	Sucrose	190627002	8
Caesar & Loretz GmbH	Sucrose	19062701	10
Caesar & Loretz GmbH	Sucrose	19062706	1
Caesar & Loretz GmbH	Sucrose	192839001	3
Caesar & Loretz GmbH	Sucrose	192839002	5
Caesar & Loretz GmbH	Sucrose	192839004	7
Caesar & Loretz GmbH	Sucrose	192839006	2
Caesar & Loretz GmbH	Sucrose	192839007	13
Caesar & Loretz GmbH	Sucrose	20004028003	11
Caesar & Loretz GmbH	Sucrose	21000656001	14
Caesar & Loretz GmbH	Sucrose	21000656006	4
Caesar & Loretz GmbH	Sucrose	21000656007	1
Caesar & Loretz GmbH	Sucrose	21000656010	8
Caesar & Loretz GmbH	Sucrose	21003804004	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Sucrose	21003804007	9
Caesar & Loretz GmbH	Sucrose	21003804012	1
Caesar & Loretz GmbH	Sucrose	21003804013	1
Caesar & Loretz Hilden	Sucrose	18257402	1
Caesar & Loretz/Noweda	Sucrose	18329702	1
Caesar und Loretz	Sucrose	18329702	1
Caleo/ Noweda	Sucrose	17106603	1
Calo, Hilden/ Phönix	Sucrose	190627002	1
Cealo	Sucrose	15446002	1
Cealo	Sucrose	16206102	1
DHU	Sucrose	7020407	1
DHU	Sucrose	9010709	1
DHU	Sucrose	9010710	1
DHU	Sucrose	9020110	1
DHU	Sucrose	9020510	1
DHU	Sucrose	9050610	1
Diamant	Sucrose	L24223	1
Euro OTC	Sucrose	12345	2
Euro OTC	Sucrose	16328605	1
Euro OTC	Sucrose	17106603	1
Euro OTC	Sucrose	17354506	1
Euro OTC	Sucrose	18024405	2
Fagron	Sucrose	1011208731	2
Fagron	Sucrose	11/16-N01	1
Fagron	Sucrose	11/16-N01	1
Fagron	Sucrose	11/20-N05	1
Fagron	Sucrose	11E19-N04	1
Fagron	Sucrose	11I16-N01	1
Fagron	Sucrose	11L09-N16	2
Fagron	Sucrose	12-E03-M01	1
Fagron	Sucrose	12E29-N04	1
Fagron	Sucrose	12G26-N01	2
Fagron	Sucrose	13A07-N03	1
Fagron	Sucrose	13D29-N08	1
Fagron	Sucrose	13G03-N16	1
Fagron	Sucrose	13G04-N01	1
Fagron	Sucrose	13I30-N05	1
Fagron	Sucrose	15446002	1
Fagron	Sucrose	16206102	1
Fagron	Sucrose	18082014D	1
Fagron	Sucrose	18257402	1
Fagron	Sucrose	2102308731	1
Fagron	Sucrose	5071201	1
Fagron	Sucrose	5112I-02207	1
Fargon	Sucrose	19I30-T05-079071	1
Gehe Weiterstadt	Sucrose	21003804012	1
Gehe	Sucrose	1434006	1
Gehe	Sucrose	15028802	1
Gehe	Sucrose	15446003	2
Gehe	Sucrose	16328607	1
GEHE	Sucrose	16328607	1
Gehe	Sucrose	17106603	1
Gehe	Sucrose	18281804	1
Gehe	Sucrose	18329702	2
Gehe	Sucrose	192839007	1
Gehe	Sucrose	21000656001	1
Gehe	Sucrose	21000656004	2
Hanns G.Werner GmbH	Sucrose	8731158	1
Haushalt	Sucrose	123456	1
Jenne	Sucrose	15182804	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Jenne	Sucrose	18257402	2
Jenne	Sucrose	24000032005	1
Kaufland	Sucrose	L24475	1
Kaufland	Sucrose	L24494	2
Kehr	Sucrose	16328606	1
Kehr	Sucrose	190627002	1
L12	Sucrose	18154603	1
Lebensmittelware (Edeka)	Sucrose		1
Noweda	Sucrose	13352920	2
Noweda	Sucrose	16328603	1
Noweda	Sucrose	16328607	1
Noweda	Sucrose	18154603	1
Noweda	Sucrose	220002704004	1
Penny Markt	Sucrose	201L113530100	3
Penny Markt	Sucrose	L120325600	2
Penny Markt	Sucrose	L120404100	3
Penny Markt	Sucrose	L120612100	3
Penny Markt	Sucrose	L120628000	3
Penny	Sucrose	L12513800	3
Pfeifer/Langen	Sucrose	L03144N	1
Pharmachem	Sucrose	7878	1
pharm-a-speres	Sucrose	8731003	1
pharm-a-spheres/sana…	Sucrose	8731306	1
Phoenix	Sucrose	18257402	1
Phoenix	Sucrose	190627002	2
Phoenix	Sucrose	192839004	1
phoenix	Sucrose	2100656001	1
Phönix	Sucrose	15446002	1
phönix	Sucrose	16351701	1
PHÖNIX	Sucrose	17106603	1
Phönix	Sucrose	18154603	3
Phönix	Sucrose	192839004	2
ROHA	Sucrose	130090	1
Salvator Apotheke	Sucrose	R2229455M	1
Sanacorp/Caela	Sucrose	17106603	1
Sanacorp	Sucrose	14197301	1
Sanacorp	Sucrose	14340005	1
Sanacorp	Sucrose	17106603	1
Sanacorp	Sucrose	192839007	1
Sanacorp	Sucrose	22002704004	1
Sanacorp	Sucrose	23000893002	1
Sanacorp	Sucrose	AKD5	1
Soldan	Sucrose		1
Soldan	Sucrose	232027	1
Soldan	Sucrose	243983	1
Spagyra Österreich	Sucrose	15112321097	1
Spagyra Österreich	Sucrose	21102920359	1
Spagyra/Österreich	Sucrose	10070521044	1
Spagyra/Österreich	Sucrose	12112721050	1
Spagyra/Österreich	Sucrose	13021920149	1
Spagyra/Österreich	Sucrose	13050621774	1
Spagyra/Österreich	Sucrose	13091920456	1
Spagyra/Österreich	Sucrose	13102520353	1
Spagyra/Österreich	Sucrose	13111121193	1
Spagyra/Österreich	Sucrose	14010721509	1
Spagyra/Österreich	Sucrose	14012420377	1
Spagyra/Österreich	Sucrose	14041421810	1
Spagyra/Österreich	Sucrose	14050621091	1
Spagyra/Österreich	Sucrose	14060353342	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Spagyra/Österreich	Sucrose	14060353343	1
Spagyra/Österreich	Sucrose	14070721041	1
Spagyra/Österreich	Sucrose	14071421137	2
Spagyra/Österreich	Sucrose	16122820921	1
Spagyra/Österreich	Sucrose	1624	1
Spagyra/Österreich	Sucrose	17020820810	1
Spagyra/Österreich	Sucrose	17020820816	1
Spagyra/Österreich	Sucrose	17021620307	1
Spagyra/Österreich	Sucrose	17021620309	1
Spagyra/Österreich	Sucrose	17022022188	1
Spagyra/Österreich	Sucrose	17032120927	1
Spagyra/Österreich	Sucrose	17032321132	1
Spagyra/Österreich	Sucrose	17032820797	1
Spagyra/Österreich	Sucrose	17041821026	1
Spagyra/Österreich	Sucrose	17041821027	1
Spagyra/Österreich	Sucrose	17070320627	1
Spagyra/Österreich	Sucrose	17091520139	1
Spagyra/Österreich	Sucrose	17092620773	1
Spagyra/Österreich	Sucrose	17121420710	1
Spagyra/Österreich	Sucrose	1721420709	1
Spagyra/Österreich	Sucrose	18021921250	1
Spagyra/Österreich	Sucrose	18032320385	1
Spagyra/Österreich	Sucrose	18032320386	1
Spagyra/Österreich	Sucrose	18032320387	1
Spagyra/Österreich	Sucrose	18032320388	1
Spagyra/Österreich	Sucrose	18041120712	1
Spagyra/Österreich	Sucrose	18041180714	1
Spagyra/Österreich	Sucrose	18042720542	1
Spagyra/Österreich	Sucrose	18042720555	2
Spagyra/Österreich	Sucrose	18051421069	1
Spagyra/Österreich	Sucrose	18051421071	1
Spagyra/Österreich	Sucrose	18072420037	1
Spagyra/Österreich	Sucrose	18090520787	3
Spagyra/Österreich	Sucrose	18090520788	1
Spagyra/Österreich	Sucrose	18090520789	1
Spagyra/Österreich	Sucrose	18091020640	1
Spagyra/Österreich	Sucrose	18092720503	1
Spagyra/Österreich	Sucrose	1809272503	1
Spagyra/Österreich	Sucrose	18111921057	1
Spagyra/Österreich	Sucrose	18112920404	1
Spagyra/Österreich	Sucrose	18120520314	1
Spagyra/Österreich	Sucrose	18120720497	1
Spagyra/Österreich	Sucrose	18121320236	1
Spagyra/Österreich	Sucrose	18121320237	1
Spagyra/Österreich	Sucrose	19010320203	1
Spagyra/Österreich	Sucrose	19010320204	1
Spagyra/Österreich	Sucrose	19010320205	1
Spagyra/Österreich	Sucrose	19010320207	1
Spagyra/Österreich	Sucrose	19010320208	1
Spagyra/Österreich	Sucrose	19010320209	1
Spagyra/Österreich	Sucrose	19011421251	1
Spagyra/Österreich	Sucrose	19020521071	1
Spagyra/Österreich	Sucrose	19020521072	1
Spagyra/Österreich	Sucrose	19043020816	1
Spagyra/Österreich	Sucrose	19060620656	1
Spagyra/Österreich	Sucrose	19060720528	1
Spagyra/Österreich	Sucrose	19060720530	1
Spagyra/Österreich	Sucrose	19060720880	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Spagyra/Österreich	Sucrose	19062120093	1
Spagyra/Österreich	Sucrose	19071020656	1
Spagyra/Österreich	Sucrose	19071020657	1
Spagyra/Österreich	Sucrose	19071020658	1
Spagyra/Österreich	Sucrose	19071020659	1
Spagyra/Österreich	Sucrose	19080520520	1
Spagyra/Österreich	Sucrose	19080720443	1
Spagyra/Österreich	Sucrose	19082621169	1
Spagyra/Österreich	Sucrose	19082621170	1
Spagyra/Österreich	Sucrose	19082621174	1
Spagyra/Österreich	Sucrose	19082621175	1
Spagyra/Österreich	Sucrose	1910320206	1
Spagyra/Österreich	Sucrose	19110420478	1
Spagyra/Österreich	Sucrose	19110720552	1
Spagyra/Österreich	Sucrose	19112220556	1
Spagyra/Österreich	Sucrose	20012420378	1
Spagyra/Österreich	Sucrose	20012420379	1
Spagyra/Österreich	Sucrose	2001290835	1
Spagyra/Österreich	Sucrose	20021120369	1
Spagyra/Österreich	Sucrose	20021120370	1
Spagyra/Österreich	Sucrose	200220020125	1
Spagyra/Österreich	Sucrose	20022620346	1
Spagyra/Österreich	Sucrose	20022620347	1
Spagyra/Österreich	Sucrose	20030220903	1
Spagyra/Österreich	Sucrose	20030220904	1
Spagyra/Österreich	Sucrose	20030520349	1
Spagyra/Österreich	Sucrose	20030520350	1
Spagyra/Österreich	Sucrose	20031120315	1
Spagyra/Österreich	Sucrose	20031120316	1
Spagyra/Österreich	Sucrose	20031820569	1
Spagyra/Österreich	Sucrose	20032321824	1
Spagyra/Österreich	Sucrose	20032420357	1
Spagyra/Österreich	Sucrose	20032420358	1
Spagyra/Österreich	Sucrose	20032420359	1
Spagyra/Österreich	Sucrose	20032520757	1
Spagyra/Österreich	Sucrose	20032520824	1
Spagyra/Österreich	Sucrose	20032520825	1
Spagyra/Österreich	Sucrose	20032520826	1
Spagyra/Österreich	Sucrose	20032520827	1
Spagyra/Österreich	Sucrose	20033120462	1
Spagyra/Österreich	Sucrose	20040120719	1
Spagyra/Österreich	Sucrose	20040820313	1
Spagyra/Österreich	Sucrose	20040820315	1
Spagyra/Österreich	Sucrose	20042020392	2
Spagyra/Österreich	Sucrose	20042020394	1
Spagyra/Österreich	Sucrose	20042020395	1
Spagyra/Österreich	Sucrose	20042020398	1
Spagyra/Österreich	Sucrose	20042020399	1
Spagyra/Österreich	Sucrose	20042020400	1
Spagyra/Österreich	Sucrose	20042020401	1
Spagyra/Österreich	Sucrose	20042020402	1
Spagyra/Österreich	Sucrose	20050520188	1
Spagyra/Österreich	Sucrose	20050520189	1
Spagyra/Österreich	Sucrose	20050520190	1
Spagyra/Österreich	Sucrose	20050520191	1
Spagyra/Österreich	Sucrose	20050520193	1
Spagyra/Österreich	Sucrose	20050520194	1
Spagyra/Österreich	Sucrose	20050720449	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Spagyra/Österreich	Sucrose	20052520367	1
Spagyra/Österreich	Sucrose	20052520368	1
Spagyra/Österreich	Sucrose	20061720426	1
Spagyra/Österreich	Sucrose	20061720427	1
Spagyra/Österreich	Sucrose	20061720428	1
Spagyra/Österreich	Sucrose	20061720480	1
Spagyra/Österreich	Sucrose	20062620145	1
Spagyra/Österreich	Sucrose	20070720637	1
Spagyra/Österreich	Sucrose	20072920245	1
Spagyra/Österreich	Sucrose	20082620273	1
Spagyra/Österreich	Sucrose	20082620274	1
Spagyra/Österreich	Sucrose	20082820224	1
Spagyra/Österreich	Sucrose	20082820225	1
Spagyra/Österreich	Sucrose	20082820226	1
Spagyra/Österreich	Sucrose	20090120367	1
Spagyra/Österreich	Sucrose	20090120368	1
Spagyra/Österreich	Sucrose	20091020538	1
Spagyra/Österreich	Sucrose	20091020539	1
Spagyra/Österreich	Sucrose	20091720367	1
Spagyra/Österreich	Sucrose	20091720374	1
Spagyra/Österreich	Sucrose	20091720375	1
Spagyra/Österreich	Sucrose	20092821146	1
Spagyra/Österreich	Sucrose	20092821147	1
Spagyra/Österreich	Sucrose	20092821149	1
Spagyra/Österreich	Sucrose	20092821152	1
Spagyra/Österreich	Sucrose	20092821153	1
Spagyra/Österreich	Sucrose	20092821154	1
Spagyra/Österreich	Sucrose	20092821155	1
Spagyra/Österreich	Sucrose	20092821156	1
Spagyra/Österreich	Sucrose	20093020124	1
Spagyra/Österreich	Sucrose	20102320364	1
Spagyra/Österreich	Sucrose	20102320365	1
Spagyra/Österreich	Sucrose	20102320366	1
Spagyra/Österreich	Sucrose	20102720460	1
Spagyra/Österreich	Sucrose	20111720437	1
Spagyra/Österreich	Sucrose	20111720439	1
Spagyra/Österreich	Sucrose	20112321275	1
Spagyra/Österreich	Sucrose	20112321277	1
Spagyra/Österreich	Sucrose	20112321278	1
Spagyra/Österreich	Sucrose	20112321279	1
Spagyra/Österreich	Sucrose	20112520599	1
Spagyra/Österreich	Sucrose	20112520600	1
Spagyra/Österreich	Sucrose	20112520601	1
Spagyra/Österreich	Sucrose	20112520602	1
Spagyra/Österreich	Sucrose	20112520603	1
Spagyra/Österreich	Sucrose	20112520604	1
Spagyra/Österreich	Sucrose	20112520605	1
Spagyra/Österreich	Sucrose	20112520606	1
Spagyra/Österreich	Sucrose	20112520607	1
Spagyra/Österreich	Sucrose	20112520608	1
Spagyra/Österreich	Sucrose	20112520609	1
Spagyra/Österreich	Sucrose	20112720457	1
Spagyra/Österreich	Sucrose	20112720459	1
Spagyra/Österreich	Sucrose	20112720460	1
Spagyra/Österreich	Sucrose	20112720461	1
Spagyra/Österreich	Sucrose	20122320203	1
Spagyra/Österreich	Sucrose	20122320204	1
Spagyra/Österreich	Sucrose	2042220600	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Spagyra/Österreich	Sucrose	2042220601	1
Spagyra/Österreich	Sucrose	2042220602	1
Spagyra/Österreich	Sucrose	20881420115	1
Spagyra/Österreich	Sucrose	21011120754	1
Spagyra/Österreich	Sucrose	21011120755	1
Spagyra/Österreich	Sucrose	21011120756	1
Spagyra/Österreich	Sucrose	21012120262	1
Spagyra/Österreich	Sucrose	21022220519	1
Spagyra/Österreich	Sucrose	21022220531	1
Spagyra/Österreich	Sucrose	21022220532	1
Spagyra/Österreich	Sucrose	21022420250	1
Spagyra/Österreich	Sucrose	21030320285	1
Spagyra/Österreich	Sucrose	21030320286	1
Spagyra/Österreich	Sucrose	21030320289	1
Spagyra/Österreich	Sucrose	21031520864	1
Spagyra/Österreich	Sucrose	21031920545	1
Spagyra/Österreich	Sucrose	21033020089	1
Spagyra/Österreich	Sucrose	21042221787	1
Spagyra/Österreich	Sucrose	21042820617	1
Spagyra/Österreich	Sucrose	21050420503	1
Spagyra/Österreich	Sucrose	21051720779	1
Spagyra/Österreich	Sucrose	21051720780	1
Spagyra/Österreich	Sucrose	21051720781	1
Spagyra/Österreich	Sucrose	21051720782	1
Spagyra/Österreich	Sucrose	21051720783	1
Spagyra/Österreich	Sucrose	21051720785	1
Spagyra/Österreich	Sucrose	21051720786	1
Spagyra/Österreich	Sucrose	21061020532	1
Spagyra/Österreich	Sucrose	21061020535	1
Spagyra/Österreich	Sucrose	21072320083	1
Spagyra/Österreich	Sucrose	21072320084	2
Spagyra/Österreich	Sucrose	21090920173	1
Spagyra/Österreich	Sucrose	21090920174	1
Spagyra/Österreich	Sucrose	21090920176	2
Spagyra/Österreich	Sucrose	21090920177	2
Spagyra/Österreich	Sucrose	21101520263	1
Spagyra/Österreich	Sucrose	2307	2
Spagyra/Österreich	Sucrose	2382	1
Spagyra/Österreich	Sucrose	2506	1
Spagyra/Österreich	Sucrose	2516	1
Spagyra/Österreich	Sucrose	2963	1
Spagyra/Österreich	Sucrose	3071	1
Spagyra/Österreich	Sucrose	3082	1
Spagyra/Österreich	Sucrose	3183	1
Spagyra/Österreich	Sucrose	3303	1
Spagyra/Österreich	Sucrose	3802	1
Spagyra/Österreich	Sucrose	3988	1
Spagyra/Österreich	Sucrose	4087	1
Spagyra/Österreich	Sucrose	4153	1
Spagyra/Österreich	Sucrose	4159	1
Spagyra/Österreich	Sucrose	4251	1
Spagyra/Österreich	Sucrose	4255	1
Spagyra/Österreich	Sucrose	4338	1
Spagyra/Österreich	Sucrose	4417	1
Spagyra/Österreich	Sucrose	4504	1
Spagyra/Österreich	Sucrose	4941	1
Spagyra/Österreich	Sucrose	4965	1
Spagyra/Österreich	Sucrose	5009	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Spagyra/Österreich	Sucrose	5030920991	1
Spagyra/Österreich	Sucrose	5030920993	1
Spagyra/Österreich	Sucrose	5030921008	1
Spagyra/Österreich	Sucrose	5030921018	1
Spagyra/Österreich	Sucrose	5031	1
Spagyra/Österreich	Sucrose	5156	1
Spagyra/Österreich	Sucrose	5329	1
Spagyra/Österreich	Sucrose	5520	2
Spagyra/Österreich	Sucrose	5545	1
Spagyra/Österreich	Sucrose	5660	1
Spagyra/Österreich	Sucrose	5699	1
Spagyra/Österreich	Sucrose	5743	1
Spagyra/Österreich	Sucrose	5899	1
Spagyra/Österreich	Sucrose	5998	1
Spagyra/Österreich	Sucrose	6019	1
Spagyra/Österreich	Sucrose	6032	2
Spagyra/Österreich	Sucrose	6047	1
Spagyra/Österreich	Sucrose	6079	1
Spagyra/Österreich	Sucrose	6091	2
Spagyra/Österreich	Sucrose	6106	1
Spagyra/Österreich	Sucrose	6128	1
Spagyra/Österreich	Sucrose	6201	1
Spagyra/Österreich	Sucrose	6243	1
Spagyra/Österreich	Sucrose	6285	1
Spagyra/Österreich	Sucrose	6327	1
Spagyra/Österreich	Sucrose	6340	1
Spagyra/Österreich	Sucrose	6371	1
Spagyra/Österreich	Sucrose	6409	1
Spagyra/Österreich	Sucrose	6415	1
Spagyra/Österreich	Sucrose	6562	1
Spagyra/Österreich	Sucrose	H17-0047	1
Spagyra/Österreich	Sucrose	H18-0021	1
Spagyra/Österreich	Sucrose	H18-0210	1
Spagyra/Österreich	Sucrose	H18-0235	1
Spagyra/Österreich	Sucrose	H18-0252	1
Spagyra/Österreich	Sucrose	H18-0327	1
Spagyra/Österreich	Sucrose	H19-0130	1
Spagyra/Österreich	Sucrose	H19-0270	1
Spagyra	Sucrose	10032921256	1
Spagyra	Sucrose	10073020385	1
Spagyra	Sucrose	12082320717	1
Spagyra	Sucrose	12103020975	1
Spagyra	Sucrose	13012920302	1
Spagyra	Sucrose	13020620240	1
Spagyra	Sucrose	13030621373	1
Spagyra	Sucrose	13040921424	1
Spagyra	Sucrose	13040921427	1
Spagyra	Sucrose	13040921430	1
Spagyra	Sucrose	13040921431	1
Spagyra	Sucrose	13041920152	2
Spagyra	Sucrose	13041920154	1
Spagyra	Sucrose	13050621773	2
Spagyra	Sucrose	13051520939	1
Spagyra	Sucrose	13051520941	1
Spagyra	Sucrose	13061020524	1
Spagyra	Sucrose	13061020525	1
Spagyra	Sucrose	13061020526	1
Spagyra	Sucrose	13061020528	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Spagyra	Sucrose	13061020529	1
Spagyra	Sucrose	13061220385	2
Spagyra	Sucrose	13070420936	2
Spagyra	Sucrose	13070420937	2
Spagyra	Sucrose	13070420938	1
Spagyra	Sucrose	13072620834	1
Spagyra	Sucrose	15032620414	1
Spagyra	Sucrose	15082720411	1
Spagyra	Sucrose	16032920732	1
Spagyra	Sucrose	16042522126	1
Spagyra	Sucrose	16050220821	1
Spagyra	Sucrose	16050421023	1
Spagyra	Sucrose	16051820801	1
Spagyra	Sucrose	16053020827	1
Spagyra	Sucrose	16070421669	1
Spagyra	Sucrose	16083120745	1
Spagyra	Sucrose	16102120418	1
Spagyra	Sucrose	16110320884	1
Spagyra	Sucrose	1691	1
Spagyra	Sucrose	17070420968	1
Spagyra	Sucrose	17072120536	1
Spagyra	Sucrose	17072120537	1
Spagyra	Sucrose	17072120538	1
Spagyra	Sucrose	17080920574	1
Spagyra	Sucrose	17082320366	1
Spagyra	Sucrose	17090620617	1
Spagyra	Sucrose	18081720533	1
Spagyra	Sucrose	19043020815	1
Spagyra	Sucrose	1905	1
Spagyra	Sucrose	1911	1
Spagyra	Sucrose	1918	1
Spagyra	Sucrose	2007	2
Spagyra	Sucrose	20102720461	1
Spagyra	Sucrose	20102720462	1
Spagyra	Sucrose	2923	1
Spagyra	Sucrose	3750	1
Spagyra	Sucrose	5030920873	1
Spagyra	Sucrose	5030920881	1
Spagyra	Sucrose	5030920883	1
Spagyra	Sucrose	5030920885	1
Spagyra	Sucrose	5030920893	1
Spagyra	Sucrose	5030920895	1
Spagyra	Sucrose	5030920908	1
Spagyra	Sucrose	5030920922	1
Spagyra	Sucrose	5030920923	1
Spagyra	Sucrose	5030920924	1
Spagyra	Sucrose	5030920989	1
Spagyra	Sucrose	5030920995	1
Spagyra	Sucrose	5030920996	1
Spagyra	Sucrose	5030920997	1
Spagyra	Sucrose	5030920998	1
Spagyra	Sucrose	5030920999	1
Spagyra	Sucrose	5030921002	1
Spagyra	Sucrose	5030921004	1
Spagyra	Sucrose	5030921006	1
Spagyra	Sucrose	5030921010	1
Spagyra	Sucrose	5030921012	1
Spagyra	Sucrose	5030921014	1
Spagyra	Sucrose	5030921015	1
Spagyra	Sucrose	5030921016	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Spagyra	Sucrose	5030921019	1
Spagyra	Sucrose	5030921020	1
Spagyra	Sucrose	5030921024	1
Spagyra	Sucrose	5030921026	1
Spagyra	Sucrose	5030921028	1
Spagyra	Sucrose	5030921030	1
Spagyra	Sucrose	5030921031	1
Spagyra	Sucrose	5030921032	1
Spagyra	Sucrose	5030921036	1
Spagyra	Sucrose	5030921037	1
Spagyra	Sucrose	5030921038	1
Spagyra	Sucrose	5030921039	1
Spagyra	Sucrose	5030921040	1
Spagyra	Sucrose	5030921041	1
Spagyra	Sucrose	5030921042	1
Spagyra	Sucrose	5030921043	1
Spagyra	Sucrose	5030921053	1
Spagyra	Sucrose	5030921054	1
Spagyra	Sucrose	5030921056	1
Spagyra	Sucrose	5030921060	1
Spagyra	Sucrose	5030921064	1
Spagyra	Sucrose	5030921065	1
Spagyra	Sucrose	5030921067	1
Spagyra	Sucrose	5030921072	1
Spagyra	Sucrose	5030921075	1
Spagyra	Sucrose	5030921078	1
Spagyra	Sucrose	5030921080	1
Spagyra	Sucrose	5030921081	1
Spagyra	Sucrose	5030921082	1
Spagyra	Sucrose	5030921090	1
Spagyra	Sucrose	5030921094	1
Spagyra	Sucrose	5030921096	1
Spagyra	Sucrose	5030921100	1
Spagyra	Sucrose	5030921101	1
Spagyra	Sucrose	5030921122	1
Spagyra	Sucrose	5030921152	1
Spagyra	Sucrose	5030921221	1
Spagyra	Sucrose	7062220875	1
SpagyraÖsterreich	Sucrose	21112620135	1
SpagyraÖsterreich	Sucrose	21112620136	1
SpagyraÖsterreich	Sucrose	21112620137	1
SpagyraÖsterreich	Sucrose	21112620138	1
SpagyraÖsterreich	Sucrose	21112620139	1
SpagyraÖsterreich	Sucrose	21112620140	1
SpagyraÖsterreich	Sucrose	21112620141	1
SpagyraÖsterreich	Sucrose	21120220394	1
SpagyraÖsterreich	Sucrose	21120220395	1
SpagyraÖsterreich	Sucrose	22010420102	1
SpagyraÖsterreich	Sucrose	22010420103	1
SpagyraÖsterreich	Sucrose	22010420104	1
SpagyraÖsterreich	Sucrose	22010420105	1
SpagyraÖsterreich	Sucrose	22010420106	1
SpagyraÖsterreich	Sucrose	22010420107	1
SpagyraÖsterreich	Sucrose	22012520412	1
SpagyraÖsterreich	Sucrose	22020820910	1
SpagyraÖsterreich	Sucrose	22020820911	1
SpagyraÖsterreich	Sucrose	22020821013	1
SpagyraÖsterreich	Sucrose	22020821014	1
SpagyraÖsterreich	Sucrose	22020821015	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
SpagyraÖsterreich	Sucrose	22020821016	1
SpagyraÖsterreich	Sucrose	22021020386	1
SpagyraÖsterreich	Sucrose	22021020387	1
SpagyraÖsterreich	Sucrose	22030000141	2
SpagyraÖsterreich	Sucrose	22031720088	1
SpagyraÖsterreich	Sucrose	22042020195	1
SpagyraÖsterreich	Sucrose	22042020199	1
SpagyraÖsterreich	Sucrose	22042720155	1
SpagyraÖsterreich	Sucrose	22050620618	1
SpagyraÖsterreich	Sucrose	22050620621	2
SpagyraÖsterreich	Sucrose	22050620622	1
SpagyraÖsterreich	Sucrose	22060220035	1
SpagyraÖsterreich	Sucrose	22060220038	1
SpagyraÖsterreich	Sucrose	22060920061	1
SpagyraÖsterreich	Sucrose	22060920062	1
SpagyraÖsterreich	Sucrose	22060920063	1
SpagyraÖsterreich	Sucrose	22060920064	1
SpagyraÖsterreich	Sucrose	22060920065	1
SpagyraÖsterreich	Sucrose	22062020221	1
SpagyraÖsterreich	Sucrose	22070420262	1
SpagyraÖsterreich	Sucrose	22070820291	1
SpagyraÖsterreich	Sucrose	22080220229	1
SpagyraÖsterreich	Sucrose	22080220230	1
SpagyraÖsterreich	Sucrose	22081620115	1
SpagyraÖsterreich	Sucrose	22081620117	1
SpagyraÖsterreich	Sucrose	22083020318	1
SpagyraÖsterreich	Sucrose	22083020323	2
SpagyraÖsterreich	Sucrose	22083020326	1
SpagyraÖsterreich	Sucrose	22090220218	1
SpagyraÖsterreich	Sucrose	22090620388	1
SpagyraÖsterreich	Sucrose	6083	1
SpagyraÖsterreich	Sucrose	6116	1
SpagyraÖsterreich	Sucrose	6553	1
SpagyraÖsterreich	Sucrose	6807	1
SpagyraÖsterreich	Sucrose	680722021720173	1
SpagyraÖsterreich	Sucrose	680722021720174	1
SpagyraÖsterreich	Sucrose	680722021720175	1
SpagyraÖsterreich	Sucrose	680722021720176	1
SpagyraÖsterreich	Sucrose	680722021720177	1
SpagyraÖsterreich	Sucrose	680722021720178	1
SpagyraÖsterreich	Sucrose	7056	1
SpagyraÖsterreich	Sucrose	7075	1
SpagyraÖsterreich	Sucrose	7206	1
SpagyraÖsterreich	Sucrose	7237	1
SpagyraÖsterreich	Sucrose	7263	2
SpagyraÖsterreich	Sucrose	7318	2
SpagyraÖsterreich	Sucrose	7340	1
SpagyraÖsterreich	Sucrose	7377	1
SpagyraÖsterreich	Sucrose	7447	1
SpagyraÖsterreich	Sucrose	7656	1
SpagyraÖsterreich	Sucrose	7660	1
SpagyraÖsterreich	Sucrose	H20-0298	1
St. Erhard Apotheke	Sucrose	1809052072	1
St. Erhard Apotheke	Sucrose	18090520790	1
St. Erhard Apotheke	Sucrose	18090520791	1
St. Erhard Apotheke	Sucrose	18090520792	1
St. Erhard Apotheke	Sucrose	18090520793	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
St. Erhard Apotheke	Sucrose	18090520794	1
St. Erhard Apotheke	Sucrose	18090520795	1
St. Erhard Apotheke	Sucrose	19060720878	1
St. Erhard Apotheke	Sucrose	19061720787	1
St. Erhard Apotheke	Sucrose	19061721186	1
St. Erhard Apotheke	Sucrose	20032321403	1
St. Erhard Apotheke	Sucrose	20032321827	1
St. Erhard Apotheke	Sucrose	20100920507	1
St. Erhard Apotheke	Sucrose	21020520525	1
St. Erhard Apotheke	Sucrose	21020520526	1
St. Erhard Apotheke	Sucrose	21020520527	1
St. Erhard Apotheke	Sucrose	32520757	1
Staufen-Pharma	Sucrose	161112	2
Staufenpharma	Sucrose	3314E-01586	1
südzucker	Sucrose		1
südzucker	Sucrose	L120031600	1
Wepa	Sucrose	LOTAP-SP0005	1
Werner	Sucrose	1901208731	2

- 234 296 spectra from 1515 *Apo-Ident* customers from a total of 48 565 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sucrose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sucrose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	580	0	152 382
Type B	0	340	0	201 744
Type C	0	1771	0	234 296

The substance/substance group *Sucrose* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.9655 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.2353 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 99.6612 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21484	21484	0.00	51.55
21736	21484	4.20	54.45
22615	22615	0.00	53.90
22643	22643	0.00	57.18
23057	23057	0.00	55.10
23058	23058	0.00	56.32
23297	23297	0.00	54.56
23666	23666	0.00	57.67
23833	23833	0.00	53.22
24217	24217	0.00	58.00
25651	25651	0.00	79.97
26630	26630	0.00	58.45
26723	26723	0.00	64.00

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfacetamide**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20695-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfacetamide; Sulfacetamidum

Special notes

When selecting the *Sulfacetamide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfacetamide	6	3	38

Second-stage model

For differentiation of the substance/substance group *Sulfacetamide* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfacetamide* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Oxytetracycline hydrochloride	166.21	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfacetamide* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfacetamide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfacetamide	11085910	20695	40	1402651
Caelo	Sulfacetamide	15445901	23251	40	20160126
Caelo	Sulfacetamide	15445901	23456	40	20160126
Caelo	Sulfacetamide	20002794001	25515	40	20201022
Euro OTC	Sulfacetamide	1312012-01	21633	60	20140117
Euro OTC	Sulfacetamide	1509018	21902	60	20150929*
Euro OTC	Sulfacetamide	2101027	25546	40	20210127*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 320 spectra of 7 reference samples from the substance/substance group *Sulfacetamide*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Sulfacetamide*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Sulfacetamide	1702006	23157	40
Euro OTC	Sulfacetamide	1808035	24193	40
Euro OTC	Sulfacetamide	1907026	24804	40

- 201 964 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 184 spectra from 82 *Apo-Ident* customers from 43 batches from the substance/substance group *Sulfacetamide*.

- Among them are spectra of independent samples from 38 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
AHC 12.08.13 EK9,31	Sulfacetamide	11085912	1
Apo-ident/Alliance	Sulfacetamide	1702006-02	1
Caelo	Sulfacetamide	10145802	1
Caelo	Sulfacetamide	10145811	1
Caelo	Sulfacetamide	11085909	1
Caelo	Sulfacetamide	11085911	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sulfacetamide	11085912	4
Caelo	Sulfacetamide	11085913	2
Caelo	Sulfacetamide	11085914	2
Caelo	Sulfacetamide	11095912	1
Caelo	Sulfacetamide	1509018-02	2
Caelo	Sulfacetamide	15445901	2
Caelo	Sulfacetamide	15445902	2
Caelo	Sulfacetamide	15445904	1
Caelo	Sulfacetamide	15445905	2
Caelo	Sulfacetamide	1702006-01	1
Caelo	Sulfacetamide	20002794001	1
Caelo	Sulfacetamide	20002794002	1
Caelo	Sulfacetamide	21003927003	1
Caesar & Loretz GmbH…	Sulfacetamide	20002794002	1
Caesar & Loretz GmbH	Sulfacetamide	15445902	2
Caesar & Loretz GmbH	Sulfacetamide	20002794001	2
Caesar & Loretz GmbH	Sulfacetamide	20002794002	2
Caesar & Loretz	Sulfacetamide	15445902	1
EuRho/Jenne	Sulfacetamide	2101027-01	1
EuRho/Noweda	Sulfacetamide	1702006-04	1
EuRho/Phönix	Sulfacetamide	1702006-02	1
EuRho	Sulfacetamide	210102701	1
Euro OTC	Sulfacetamide	1112032-01	3
Euro OTC	Sulfacetamide	1112032-02	4
Euro OTC	Sulfacetamide	1312012-01	4
Euro OTC	Sulfacetamide	1312012-02	2
Euro OTC	Sulfacetamide	1509018-01	5
Euro OTC	Sulfacetamide	1509018-02	5
Euro OTC	Sulfacetamide	1509018-03	3
Euro OTC	Sulfacetamide	1702006-01	3
Euro OTC	Sulfacetamide	1702006-02	3
Euro OTC	Sulfacetamide	170200604	1
Euro OTC	Sulfacetamide	1702006-04	3
Euro OTC	Sulfacetamide	1808035-01	2
Euro OTC	Sulfacetamide	1907026	1
Euro OTC	Sulfacetamide	190702601	3
Euro OTC	Sulfacetamide	1907026-01	31
Euro OTC	Sulfacetamide	2101027	1
Euro OTC	Sulfacetamide	2101027-01	24
Euro OTC	Sulfacetamide	5119E01073	1
Euro OTC	Sulfacetamide	AP210205-03	1
Euro OTC	Sulfacetamide	AP220721-02	1
EuroRho 24.05.2013 A…	Sulfacetamide	1112032-02	2
Gehe/EuRho	Sulfacetamide	2101027-02	1
Gehe	Sulfacetamide	11085904	1
Gehe	Sulfacetamide	1112032-01	4
Gehe	Sulfacetamide	1312012-01	2
Gehe	Sulfacetamide	1312012-02	1
Gehe	Sulfacetamide	1505025-01	1
Gehe	Sulfacetamide	190702601	1
Gehe	Sulfacetamide	1907026-01	2
Gehe	Sulfacetamide	2101027-01	1
Ge-Hh	Sulfacetamide	20002794002	2
Industrias GmbH / Ph	Sulfacetamide	64518	1
Katwijk Chemie B.V.	Sulfacetamide	15445902	3
Katwijk Chemie	Sulfacetamide	1702006-01	1
Noweda	Sulfacetamide	15445904	1
Noweda	Sulfacetamide	1702006-02	1
Noweda	Sulfacetamide	2101027-01	2
Noweda200002794001	Sulfacetamide	200002794001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix 17.02.2015	Sulfacetamide	1312012-02	2
Phoenix	Sulfacetamide	15445904	1
Phönix 23.06.2014	Sulfacetamide	1312012-01	1
Phönix Gotha	Sulfacetamide	11085911	1
Phönix Gotha	Sulfacetamide	1312012-02	1
Phönix	Sulfacetamide	11085910	1
Phönix	Sulfacetamide	1509018-02	1
Phönix	Sulfacetamide	15445905	1
Phönix	Sulfacetamide	1907026-01	3
Spangropharm	Sulfacetamide	11085915	1

- 235 883 spectra from 1515 *Apo-Ident* customers from a total of 49 215 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfacetamide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfacetamide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	120	0	201 964
Type C	0	181	3	235 883

The substance/substance group *Sulfacetamide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9007 %)	98.3696 % (> 96.7391 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20695	20695	0.00	357.73
21633	21902	9.82	362.73
21902	21902	0.00	363.74
23251	21902	9.64	355.15
23456	21902	7.80	358.55
25515	21902	12.37	357.54
25546	25546	0.00	359.69

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfadiazine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20753-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfadiazine; Sulfadiazinum

Special notes

When selecting the *Sulfadiazine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfadiazine	7	6	22

Second-stage model

For differentiation of the substance/substance group *Sulfadiazine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfadiazine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	215.07	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfadiazine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfadiazine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfadiazine	12164101	20753	40	1402053
Caelo	Sulfadiazine	13150011	21744	60	20130708
Caelo	Sulfadiazine	170566	23319	40	20170330*
Caelo	Sulfadiazine	17056602	23374	40	20170330
Caelo	Sulfadiazine	17056602	23447	40	20170330
Caelo	Sulfadiazine	191850	24735	40	20190730*
Caelo	Sulfadiazine	20000240002	25513	40	20200430
Caelo	Sulfadiazine	23003071	27233	40	20240220*
Caelo	Sulfadiazine	23003071	27233SI	20	20240220*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Sulfadiazine*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 602 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 260 spectra of 8 reference samples from the substance/substance group *Sulfadiazine*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sulfadiazine	172222	23630	30
Caelo	Sulfadiazine	190683	24523	40
Caelo	Sulfadiazine	21002176001	26412	40
Caelo	Sulfadiazine	24001426	27325	40
Fagron	Sulfadiazine	21G10-B22-216650	26061	40
Fagron	Sulfadiazine	23G05-B11-231251	27064	40
Fagron	Sulfadiazine	21G10-B22-216650	26061SI	10
Fagron	Sulfadiazine	23G05-B11-231251	27064SI	20

- 201 824 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 48 spectra from 23 *Apo-Ident* customers from 23 batches from the substance/substance group *Sulfadiazine*.

- Among them are spectra of independent samples from 22 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Sulfadiazine	11194204	1
Caelo	Sulfadiazine	13150004	1
Caelo	Sulfadiazine	17358901	1
Caelo	Sulfadiazine	17358905	2
Caelo	Sulfadiazine	17358906	1
Caelo	Sulfadiazine	17358910	4
Caelo	Sulfadiazine	17358913	1
Caelo	Sulfadiazine	17358917	1
Caelo	Sulfadiazine	19068302	3
Caelo	Sulfadiazine	191850001	2
Caelo	Sulfadiazine	191850002	2
Caelo	Sulfadiazine	20000240002	4
Caelo	Sulfadiazine	20000240003	6
Caelo	Sulfadiazine	2000024002	2
Caelo	Sulfadiazine	200024003	1
Caelo	Sulfadiazine	20003569003	4
Caelo	Sulfadiazine	21002176001	1
Caelo	Sulfadiazine	21002176002	1
Caelo	Sulfadiazine	240002	1
Caesar & Loretz GmbH	Sulfadiazine	19068301	1
Caesar & Loretz GmbH	Sulfadiazine	19068302	1
Caesar & Loretz GmbH	Sulfadiazine	20000240005	2
Caesar & Loretz GmbH	Sulfadiazine	20000240006	1
Caesar & Loretz GmbH	Sulfadiazine	20003569002	1
Caesar & Loretz GmbH	Sulfadiazine	20003569003	3

- 236 019 spectra from 1515 *Apo-Ident* customers from a total of 49 235 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfadiazine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfadiazine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	260	0	201 824
Type C	0	48	0	236 019

The substance/substance group *Sulfadiazine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.6923 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 87.5000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20753	20753	0.00	426.89
21744	23319	7.00	431.46
23319	23319	0.00	431.44
23374	23319	6.08	430.23
23447	23319	4.74	431.09
24735	24735	0.00	432.03
25513	20753	8.58	430.93
27233	27233	0.00	429.67

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulfogaiacol hydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20327-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulfogaiacol hydrate; Potassium guaiacolsulfonate; Sulfoguaiacolum hydricum

Special notes

When selecting the *Sulfogaiacol hydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulfogaiacol hydrate	6	2	1

Second-stage model

For differentiation of the substance/substance group *Sulfogaiacol hydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulfogaiacol hydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	71.83	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulfogaiacol hydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulfogaiacol hydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Sulfogaiacol hydrate	13405805	21696	45	20140108
Caelo	Sulfogaiacol hydrate	190303	24495	40	20190222*
Caelo	Sulfogaiacol hydrate	20001657	25191	40	20200619*
Gatt-Koller	Sulfogaiacol hydrate	1156/04152115	21843	60	20150410
Gatt-Koller	Sulfogaiacol hydrate	4543/01170317	23113	40	AR-17-FG-012520-01
Gatt-Koller	Sulfogaiacol hydrate	23J00290	26680	40	20230314
Gatt-Koller	Sulfogaiacol hydrate	23J00290	26680SI	20	20230314

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 285 spectra of 7 reference samples from the substance/substance group *Sulfogaiacol hydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 677 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 120 spectra of 3 reference samples from the substance/substance group *Sulfogaiacol hydrate*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Sulfogaiacol hydrate	170919	23300	40
Caelo	Sulfogaiacol hydrate	190921	24732	40
Caelo	Sulfogaiacol hydrate	170919	23306	40

- 201 964 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 12 spectra from 4 *Apo-Ident* customers from 1 batches from the substance/substance group *Sulfogaiacol hydrate*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Sulfogaiacol hydrate	15343912	12

- 236 055 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are docu-

mented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulfogaiacol hydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulfogaiacol hydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	285	0	152 677
Type B	0	120	0	201 964
Type C	0	12	0	236 055

The substance/substance group *Sulfogaiacol hydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8947 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.0000 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21696	23113	22.13	203.29
21843	23113	26.71	198.83
23113	23113	0.00	213.28
24495	24495	0.00	207.22
25191	25191	0.00	221.38
26680	25191	25.76	214.01

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Sulpiride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10005288-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Sulpiride; Sulpiridum

Special notes

When selecting the *Sulpiride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Sulpiride	2	3	0

Second-stage model

For differentiation of the substance/substance group *Sulpiride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Sulpiride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	151.54	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Sulpiride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Sulpiride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Sulpiride	20I16-F01-374539	26320	40	230502387
Fagron	Sulpiride	20I16-F01-374539	26320SI	20	230502387
Pharma Che…	Sulpiride	21F16-1226	26318	40	20210616
Pharma Che…	Sulpiride	21F16-1226	26318SI	20	20210616

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 120 spectra of 4 reference samples from the substance/substance group *Sulpiride*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.
- 152 842 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 4 reference samples from the substance/substance group *Sulpiride*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Sulpiride	18H09-B08-355949	25692	50
FSA Chemicals	Sulpiride	19G29-APR90102	25693	50
FSA Chemicals	Sulpiride	21G16-APR21165	26319	40
FSA Chemicals	Sulpiride	21G16-APR21165	26319SI	20

- 201 924 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Sulpiride*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Sulpiride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Sulpiride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	120	0	152 842
Type B	0	160	0	201 924
Type C	0	0	0	236 067

The substance/substance group *Sulpiride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26318	26320	36.13	236.06
26320	26320	0.00	236.60

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tacrolimus monohydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10005936-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tacrolimus monohydrate ; Tacrolimusum monohydricum

Special notes

When selecting the *Tacrolimus monohydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tacrolimus monohydrate	4	3	1

Second-stage model

For differentiation of the substance/substance group *Tacrolimus monohydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tacrolimus monohydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	99.09	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tacrolimus monohydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tacrolimus monohydrate* :

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Tacrolimus monohydrate	2201007	25941	40	20220301*
Euro OTC	Tacrolimus monohydrate	2205032	26417	30	20221110*
Fagron	Tacrolimus monohydrate	21I24-B12-215778	26147	40	20211223
Fagron	Tacrolimus monohydrate	21I24-B12-215778	26147SI	20	20211223
Fagron	Tacrolimus monohydrate	23K23-B05-223469	27048	40	20231229

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 170 spectra of 5 reference samples from the substance/substance group *Tacrolimus monohydrate* . These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 792 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 150 spectra of 5 reference samples from the substance/substance group *Tacrolimus monohydrate* .

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Tacrolimus monohydrate	1904015	24605	40
Euro OTC	Tacrolimus monohydrate	2304013	26762	40
Euro OTC	Tacrolimus monohydrate	2405003	27360	40
Euro OTC	Tacrolimus monohydrate	2201007	25941SI†	10
Euro OTC	Tacrolimus monohydrate	2304013	26762SI	20

- 201 934 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 3 spectra from 2 *Apo-Ident* customers from 1 batches from the substance/substance group *Tacrolimus monohydrate* .

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tacrolimus monohydrate	2304013-01	2
Euro OTC	Tacrolimus monohydrate	2304013-01	1

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- 236 064 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tacrolimus monohydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tacrolimus monohydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	170	0	152 792
Type B	0	150	0	201 934
Type C	0	3	0	236 064

The substance/substance group *Tacrolimus monohydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.4706 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.0000 %)
Type C	100.0000 % (> 99.9011 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
25941	25941	0.00	146.02
26147	25941	20.68	149.00
26417	26417	0.00	150.16
27048	26417	21.25	150.85

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tannin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20018-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tannin; Tanninum

Special notes

When selecting the *Tannin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tannin	6	3	154

Second-stage model

For differentiation of the substance/substance group *Tannin* the following second-stage model is used:

- Submodel 09

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tannin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	54.53	–
⋮	⋮	⋮
Dequalinium chloride	>50	48.63
Oxytetracycline hydrochloride	>50	72.35
Levothyroxin sodium	>50	95.27
Eosin Y	>50	95.87
Dithranol	>50	489.15
Acetylsalicylic acid	>50	539.60
Sodium salicylate	>50	709.01
Benzoic acid	>50	1074.05

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tannin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tannin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Tannin	12336016	21608	60	20121127
Caelo	Tannin	172092	23631	40	20170829*
Caelo	Tannin	20002512002	25516	40	20200904
Caelo	Tannin	22001643	26254	40	20220613*
Fagron	Tannin	13H30-B03-287645	21653	60	1711482
Fagron	Tannin	16D08-B04-328410	23211	40	AR-17-FG-015963-01
Fagron	Tannin	16D08-B04-328410	23501	40	20160425

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 320 spectra of 7 reference samples from the substance/substance group *Tannin*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 5 reference samples from the substance/substance group *Tannin*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Tannin	16074504	23205	40
Fagron	Tannin	20F16-B04-203751	25751	50
Fagron	Tannin	21C15-B08-210552	25902	40
Caelo	Tannin	22001643	26254SI†	20
Fagron	Tannin	21C15-B08-210552	25902SI	40

- 201 894 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 618 spectra from 373 *Apo-Ident* customers from 160 batches from the substance/substance group *Tannin*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 153 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tannin	20F16-B04-203751	1
	Tannin	21C15-B08-210552	2
	Tannin	22001643003	2
	Tannin	22001643011	4
A.H.D.	Tannin	13E27-N08	1
AHC	Tannin	20004500007	1
ALH	Tannin	14031919	1
ALH	Tannin	15091515	1
Alliance Healthcare	Tannin	12336001	1
Alliance	Tannin	200004500002	1
Caelo	Tannin		1
Caelo	Tannin	10019007	1
Caelo	Tannin	10315107	2
Caelo	Tannin	10315110	2
Caelo	Tannin	1091503	1
Caelo	Tannin	11302307	5
Caelo	Tannin	12171101	4
Caelo	Tannin	12171103	2
Caelo	Tannin	12171106	7
Caelo	Tannin	1217112263904	1
Caelo	Tannin	12336001	11
Caelo	Tannin	12336005	2
Caelo	Tannin	12336007	2
Caelo	Tannin	12336009	10
Caelo	Tannin	12336011	1
Caelo	Tannin	12336013	5
Caelo	Tannin	12336014	5
Caelo	Tannin	12336016	7
Caelo	Tannin	1236001	1
Caelo	Tannin	12A27-N01	1
Caelo	Tannin	13031401	1
Caelo	Tannin	14031901	2
Caelo	Tannin	14031903	5
Caelo	Tannin	14031905	3
Caelo	Tannin	14031912	4
Caelo	Tannin	14031913	2
Caelo	Tannin	14031915	2
Caelo	Tannin	14031918	4
Caelo	Tannin	14031919	6
Caelo	Tannin	14031920	2
Caelo	Tannin	15091503	3
Caelo	Tannin	15091504	4
Caelo	Tannin	15091506	1
Caelo	Tannin	15091509	18
Caelo	Tannin	15091511	2
Caelo	Tannin	15091512	1
Caelo	Tannin	15091515	15
Caelo	Tannin	1509509	1
Caelo	Tannin	1524308	1
Caelo	Tannin	15243801	11
Caelo	Tannin	15243802	3
Caelo	Tannin	15F23-B01-326357	1
Caelo	Tannin	16074504	15
Caelo	Tannin	16074505	1
Caelo	Tannin	16074507	1
Caelo	Tannin	16074509	8
Caelo	Tannin	16074509/171027T	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tannin	16074516	13
Caelo	Tannin	16074517	1
Caelo	Tannin	16074518	8
Caelo	Tannin	16D08-B04-328410	1
Caelo	Tannin	16D08-B04-334834	1
Caelo	Tannin	16D08-B04-354470	1
Caelo	Tannin	17343502	1
Caelo	Tannin	17343503	1
Caelo	Tannin	17343504	13
Caelo	Tannin	17343505	1
Caelo	Tannin	17343509	8
Caelo	Tannin	17343511	2
Caelo	Tannin	17343515	13
Caelo	Tannin	17343518	1
Caelo	Tannin	17343519	1
Caelo	Tannin	17343520	12
Caelo	Tannin	1734515	1
Caelo	Tannin	18017701	6
Caelo	Tannin	191382001	1
Caelo	Tannin	191382002	2
Caelo	Tannin	191382003	1
Caelo	Tannin	191382006	19
Caelo	Tannin	191382007	2
Caelo	Tannin	19138202	5
Caelo	Tannin	19138203	16
Caelo	Tannin	19138204	1
Caelo	Tannin	20002512002	23
Caelo	Tannin	20004500002	17
Caelo	Tannin	20004500007	7
Caelo	Tannin	20004500011	3
Caelo	Tannin	20045000007	1
Caelo	Tannin	21101305	1
Caelo	Tannin	22001643003	4
Caelo	Tannin	22001643011	1
Caelo	Tannin	2211Q-01052	1
Caelo	Tannin	28011502	1
Caelo	Tannin	318E-01052	1
Caelo	Tannin	320E01052	1
Caelo	Tannin	3513A-01052	1
Caelo	Tannin	41161-01052	1
Caelo	Tannin	4413I1052	1
Caelo	Tannin	70132238	1
Caelo	Tannin	9128607	2
Caelo	Tannin	9128608	1
Caelo	Tannin	91382031	1
Caelo	Tannin	B01-326357	1
Caelo	Tannin	B04-1976109	1
Caelo	Tannin	B04-2037501	1
Caelo	Tannin	Tannin20004500002	1
Caeol/ Noweda	Tannin	16074505	1
Caesar & Loretz GmbH...	Tannin	19138203	1
Caesar & Loretz GmbH...	Tannin	191382006	1
Caesar & Loretz GmbH...	Tannin	20004500002	1
Caesar & Loretz GmbH...	Tannin	191382006	1
Caesar & Loretz GmbH...	Tannin	20004500003	1
Caesar & Loretz GmbH...	Tannin	20004500002	1
Caesar & Loretz GmbH...	Tannin	191382006	1
Caesar & Loretz GmbH...	Tannin	17343520	1
Caesar & Loretz GmbH...	Tannin	20002512002	1
Caesar & Loretz GmbH...	Tannin	20002512003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Tannin	20004500002	1
Caesar & Loretz GmbH/Otto	Tannin	20002512002	1
Caesar & Loretz GmbH...	Tannin	20004500002	1
Caesar & Loretz GmbH...	Tannin	20004500002	1
Caesar & Loretz GmbH...	Tannin	200004500001	1
Caesar & Loretz GmbH...	Tannin	20004500002	1
Caesar & Loretz GmbH	Tannin	16D08-B04	1
Caesar & Loretz GmbH	Tannin	17343509	1
Caesar & Loretz GmbH	Tannin	17343515	2
Caesar & Loretz GmbH	Tannin	17343520	6
Caesar & Loretz GmbH	Tannin	191382006	5
Caesar & Loretz GmbH	Tannin	191382007	1
Caesar & Loretz GmbH	Tannin	19138202	1
Caesar & Loretz GmbH	Tannin	19138203	3
Caesar & Loretz GmbH	Tannin	20002512001	1
Caesar & Loretz GmbH	Tannin	20002512002	5
Caesar & Loretz GmbH	Tannin	20004500002	10
Caesar & Loretz GmbH	Tannin	20F16-B04-197619	1
Caesar & Loretz	Tannin	16074504	1
Caesar Loretz	Tannin	20002512002	1
Caesar/Lorenz	Tannin	11302307	1
Caleo/Phoenix	Tannin	14K17-B08-306993	1
Ebert u. Jacobi 1...	Tannin	15091509	1
Euro OTC	Tannin	15091509	1
Euro OTC	Tannin	16074501	1
Euro OTC	Tannin	16074509	1
Euro OTC	Tannin	18017701	1
Euro OTC	Tannin	4117I-01052	1
Fagron	Tannin	1014A-01052	1
Fagron	Tannin	11C09-N05	1
Fagron	Tannin	12A27-N01	1
Fagron	Tannin	12E21-N04	4
Fagron	Tannin	12H14N05	1
Fagron	Tannin	12H14-N05	5
Fagron	Tannin	13B28-N08	1
Fagron	Tannin	13E27-N08	1
Fagron	Tannin	13H30-B03287645	1
Fagron	Tannin	13H30-B03-287645	2
Fagron	Tannin	14A07-B01-293468	5
Fagron	Tannin	14e07-b03-298480	1
Fagron	Tannin	14E07-B03-298480	2
Fagron	Tannin	14J06-B04	1
Fagron	Tannin	14J06-B04-0858	1
Fagron	Tannin	14J06B04299398	2
Fagron	Tannin	14J06-B04-299398	2
Fagron	Tannin	14K17-B08-306993	1
Fagron	Tannin	15F23-B01	1
Fagron	Tannin	15F23-B01-322984	3
Fagron	Tannin	15F23B01326357	1
Fagron	Tannin	15F23-B01-326357	1
Fagron	Tannin	160300029	1
Fagron	Tannin	160300126	1
Fagron	Tannin	160300146	2
Fagron	Tannin	1603001788	1
Fagron	Tannin	160300178B	3
Fagron	Tannin	163001788	1
Fagron	Tannin	16D08-b04	1
Fagron	Tannin	16D08B04	2
Fagron	Tannin	16D08-B04	2
Fagron	Tannin	16D08-B04-328410	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Tannin	16D08-B04-334834	3
Fagron	Tannin	16D08B04335787	1
Fagron	Tannin	16D08-B04-335787	2
Fagron	Tannin	16D08-B04-337161	1
Fagron	Tannin	16D08-B04-352128	3
Fagron	Tannin	16D08-B04-354470	3
Fagron	Tannin	16D08B04354470	1
Fagron	Tannin	20F16-B04	1
Fagron	Tannin	20F16-B04-197619	8
Fagron	Tannin	20F16-B04-2033751	2
Fagron	Tannin	20F16-B04-203751	10
Fagron	Tannin	20F16-bo4-203751	1
Fagron	Tannin	21C15-B08	1
Fagron	Tannin	21C15-B08-210552	5
Fagron	Tannin	21C5-B08-210552	1
Fagron	Tannin	2212M-01052	1
Fagron	Tannin	2DF16-B04-203751	1
Fagron	Tannin	3518M-01052	1
Fagron	Tannin	4-20375001	1
Fagron	Tannin	B04-2037501	2
Fiebig	Tannin	16074518	1
Frago/Gehe	Tannin	15F23-B01	1
Gatt-Koller / Phoenix	Tannin	3335/08134613	1
Gatt-Koller / Phoenix	Tannin	333508134613	2
Gehe	Tannin	12171106	1
Gehe	Tannin	12336016	2
Gehe	Tannin	12H14-N05	1
Gehe	Tannin	15091506	1
Gehe	Tannin	16074504	1
Gehe	Tannin	20002512002	1
Gehe	Tannin	20004500002	1
Gehe	Tannin	21C15-B08-210552	1
Hirsch	Tannin	1811209	1
INTERN-DROGEN	Tannin	20004500002	1
Kehr	Tannin	22001643011	1
L10	Tannin	17343509	1
Nachprüfung	Tannin	5210A-01052	1
Noweda	Tannin	16074509	1
Noweda	Tannin	17343520	1
Noweda	Tannin	191382006	1
Phoenix	Tannin	12336013	1
Phoenix	Tannin	16074509	1
Phönix	Tannin	10313107Retest	1
Phönix	Tannin	10315110	1
phönix	Tannin	14E07-B03-293744	1
phönix	Tannin	15/AKD65	1
Phönix	Tannin	17343520	1
Sanacorp WE: 26.01.1…	Tannin	14031912	1
Sanacorp	Tannin		1
Sanacorp	Tannin	12171102	1
Sanacorp	Tannin	12336011	1
Sanacorp	Tannin	12336014	1
Sanacorp	Tannin	14031912	1
Sanacorp	Tannin	16D08-B04	1
Sanacorp	Tannin	21C15-B08-210552	1
Sanacorp	Tannin	22001613011	2
Sanacorp	Tannin	22001643003	1
Synopharm/Anzag	Tannin	3411I-01052	1

- 235 449 spectra from 1515 *Apo-Ident* customers from a total of 49 100 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tannin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tannin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	190	0	201 894
Type C	0	602	16	235 449

The substance/substance group *Tannin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9007 %)	97.4110 % (> 96.9256 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21608	23211	46.90	126.76
21653	21653	0.00	119.38
23211	23211	0.00	131.90
23501	23211	8.96	128.99
23631	23631	0.00	111.66
25516	23211	21.95	134.19
26254	26254	0.00	116.12

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tartaric acid**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20014-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tartaric acid; Acidum tartaricum

Special notes

When selecting the *Tartaric acid* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tartaric acid	10	4	172

Second-stage model

For differentiation of the substance/substance group *Tartaric acid* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tartaric acid* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	87.05	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tartaric acid* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tartaric acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Tartaric acid	15130201	22383	60	20150416
Caelo	Tartaric acid	15164001	22384	60	1704461
Caelo	Tartaric acid	161468	22613	40	20160607*
Caelo	Tartaric acid	21000301	25628	40	20210301*
Caelo	Tartaric acid	21000938	25699	50	20210430*
Caelo	Tartaric acid	24001998	27307	40	20240906*
Caelo	Tartaric acid	24001998	27307SI	20	20240906*
Euro OTC	Tartaric acid	1907022	24806	40	20190813*
Fagron	Tartaric acid	13I25-B01-294093	22391	60	1711509
Fagron	Tartaric acid	14G07-B02-308554	22501	40	20140827
Fagron	Tartaric acid	21J15-B03-220487	26397	40	20220126
Fagron	Tartaric acid	21J15-B03-220487	26397SI	20	20220126

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 510 spectra of 12 reference samples from the substance/substance group *Tartaric acid*. These samples are listed above in the *calibration samples* section. The reference samples come from 10 different batches.

- 152 452 spectra from a total of 2832 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 4 reference samples from the substance/substance group *Tartaric acid*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Tartaric acid	13217803	21457	60
Caelo	Tartaric acid	181212	24015	40
Caelo	Tartaric acid	21002221	25799	50
Fagron	Tartaric acid	14G07-B02-322976	23527	40

- 201 894 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 440 spectra from 210 *Apo-Ident* customers from 180 batches from the substance/substance group *Tartaric acid*.

- Among them are spectra of independent samples from 171 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tartaric acid	20J05B01202754	1
	Tartaric acid	21000301006	1
	Tartaric acid	23000312004	1
apomix	Tartaric acid		1
apomix	Tartaric acid	1111	1
Beiersdorf AG	Tartaric acid	11G19-N08	2
Caelo	Tartaric acid		1
Caelo	Tartaric acid	10073105	1
Caelo	Tartaric acid	10180708	2
Caelo	Tartaric acid	10180713	2
Caelo	Tartaric acid	10180714	1
Caelo	Tartaric acid	10199713	1
Caelo	Tartaric acid	11169406	2
Caelo	Tartaric acid	1169406	1
Caelo	Tartaric acid	11k10-n07	1
Caelo	Tartaric acid	1204102	1
Caelo	Tartaric acid	12044101	2
Caelo	Tartaric acid	12044102	3
Caelo	Tartaric acid	12044103	4
Caelo	Tartaric acid	12044119	3
Caelo	Tartaric acid	12240402	1
Caelo	Tartaric acid	12240413	1
Caelo	Tartaric acid	12240415	1
Caelo	Tartaric acid	12286903	2
Caelo	Tartaric acid	12286904	2
Caelo	Tartaric acid	12286906	4
Caelo	Tartaric acid	12286911	1
Caelo	Tartaric acid	12286924	1
Caelo	Tartaric acid	12286932	1
Caelo	Tartaric acid	12286934	1
Caelo	Tartaric acid	12286939	1
Caelo	Tartaric acid	12H02-n07	1
Caelo	Tartaric acid	13116306	1
Caelo	Tartaric acid	13116307	1
Caelo	Tartaric acid	13116308	2
Caelo	Tartaric acid	13217803	1
Caelo	Tartaric acid	13217806	2
Caelo	Tartaric acid	13217807	1
Caelo	Tartaric acid	13B15-N01	2
Caelo	Tartaric acid	13125-B01-294093	1
Caelo	Tartaric acid	14054521	1
Caelo	Tartaric acid	14186211	1
Caelo	Tartaric acid	14186213	4
Caelo	Tartaric acid	14G07-B02-308555	2
Caelo	Tartaric acid	14G07-B02-330640	1
Caelo	Tartaric acid	15045303	1
Caelo	Tartaric acid	15045304	1
Caelo	Tartaric acid	151302	1
Caelo	Tartaric acid	15130201	6
Caelo	Tartaric acid	15130205	2
Caelo	Tartaric acid	15130206	1
Caelo	Tartaric acid	15130207	1
Caelo	Tartaric acid	15164001	4
Caelo	Tartaric acid	15164002	3
Caelo	Tartaric acid	15164008	5
Caelo	Tartaric acid	15164010	1
Caelo	Tartaric acid	15349101	5
Caelo	Tartaric acid	15349102	5
Caelo	Tartaric acid	15349105	9
Caelo	Tartaric acid	15349106	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tartaric acid	15349109	5
Caelo	Tartaric acid	15349110	2
Caelo	Tartaric acid	16146806	2
Caelo	Tartaric acid	16146809	1
Caelo	Tartaric acid	16146811	1
Caelo	Tartaric acid	16260403	5
Caelo	Tartaric acid	16260404	5
Caelo	Tartaric acid	16260405	1
Caelo	Tartaric acid	16260406	5
Caelo	Tartaric acid	17091402	1
Caelo	Tartaric acid	17337504	2
Caelo	Tartaric acid	17337505	3
Caelo	Tartaric acid	17337506	2
Caelo	Tartaric acid	17347103	5
Caelo	Tartaric acid	17347104	3
Caelo	Tartaric acid	1812104	1
Caelo	Tartaric acid	18121201	1
Caelo	Tartaric acid	18121204	6
Caelo	Tartaric acid	18121205	1
Caelo	Tartaric acid	18121208	6
Caelo	Tartaric acid	18121210	5
Caelo	Tartaric acid	18121211	9
Caelo	Tartaric acid	18121212	3
Caelo	Tartaric acid	18121214	9
Caelo	Tartaric acid	182394004	1
Caelo	Tartaric acid	18239403	1
Caelo	Tartaric acid	18239405	1
Caelo	Tartaric acid	18239406	3
Caelo	Tartaric acid	18239407	3
Caelo	Tartaric acid	18239407/P-04121921	1
Caelo	Tartaric acid	191825002	10
Caelo	Tartaric acid	191825003	13
Caelo	Tartaric acid	191825004	2
Caelo	Tartaric acid	191825006	2
Caelo	Tartaric acid	19182502	1
Caelo	Tartaric acid	19825005	1
Caelo	Tartaric acid	21000301001	2
Caelo	Tartaric acid	21000938002	3
Caelo	Tartaric acid	21000938004	1
Caelo	Tartaric acid	21000938006	1
Caelo	Tartaric acid	21000938007	2
Caelo	Tartaric acid	21000938008	1
Caelo	Tartaric acid	21002221001	1
Caelo	Tartaric acid	2717I-01053	1
Caelo	Tartaric acid	4110N-01053	1
Caelo	Tartaric acid	708061	2
Caelo	Tartaric acid	8051809	1
Caelo	Tartaric acid	9041703	1
Caelo	Tartaric acid	9494239	1
Caesar & Loretz GmbH...	Tartaric acid	17337504	2
Caesar & Loretz GmbH...	Tartaric acid	18239405	1
Caesar & Loretz GmbH...	Tartaric acid	18121211	1
Caesar & Loretz GmbH...	Tartaric acid	191825003	1
Caesar & Loretz GmbH/Gehe	Tartaric acid	18121211	1
Caesar & Loretz GmbH/Gehe	Tartaric acid	18121214	1
Caesar & Loretz GmbH/Gehe	Tartaric acid	191825002	3
Caesar & Loretz GmbH/Gehe	Tartaric acid	9494222	1
Caesar & Loretz GmbH...	Tartaric acid	191825004	1
Caesar & Loretz GmbH...	Tartaric acid	182394004	1
Caesar & Loretz GmbH...	Tartaric acid	18239405	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Tartaric acid	17337505	1
Caesar & Loretz GmbH...	Tartaric acid	18121212	1
Caesar & Loretz GmbH	Tartaric acid	18121204	1
Caesar & Loretz GmbH	Tartaric acid	18121208	3
Caesar & Loretz GmbH	Tartaric acid	18121210	1
Caesar & Loretz GmbH	Tartaric acid	18121211	1
Caesar & Loretz GmbH	Tartaric acid	18239405	1
Caesar & Loretz GmbH	Tartaric acid	18239406	1
Caesar & Loretz GmbH	Tartaric acid	191825002	3
Caesar & Loretz GmbH	Tartaric acid	191825003	7
Caesar & Loretz GmbH	Tartaric acid	191825004	3
Caesar & Loretz GmbH	Tartaric acid	191825005	2
Caesar & Loretz GmbH	Tartaric acid	19182501	1
Caesar & Loretz GmbH	Tartaric acid	21000938003	3
Caesar & Loretz/ Noweda	Tartaric acid	12044103	1
canea, anzag	Tartaric acid	12286906	1
Distillerie Mazzari/...	Tartaric acid	13405	1
E-plus	Tartaric acid	15349107	1
Euro OTC	Tartaric acid	1604046-02	1
Euro OTC	Tartaric acid	17347103	1
Euro OTC	Tartaric acid	702265	1
Fagron	Tartaric acid	1106211053	1
Fagron	Tartaric acid	11E24-N06	1
Fagron	Tartaric acid	11E24-N060752/764	1
Fagron	Tartaric acid	12131	2
Fagron	Tartaric acid	12225	1
Fagron	Tartaric acid	12F18-N02	1
Fagron	Tartaric acid	12F18-No2	1
Fagron	Tartaric acid	12H02-N07	3
Fagron	Tartaric acid	12K16-N02	1
Fagron	Tartaric acid	12K29-B01-285247	1
Fagron	Tartaric acid	13/25-B01	1
Fagron	Tartaric acid	13/25-B01-285487	1
Fagron	Tartaric acid	13/25-B01-285488	2
Fagron	Tartaric acid	13/25-B01-294094	1
Fagron	Tartaric acid	1325-B01-294093	1
Fagron	Tartaric acid	1325-B01-294094	1
Fagron	Tartaric acid	13B15N01	1
Fagron	Tartaric acid	13B15-N01	8
Fagron	Tartaric acid	13G03-N14	1
Fagron	Tartaric acid	13I25-B01	1
Fagron	Tartaric acid	13I25-B01-285487	1
Fagron	Tartaric acid	13I25-B01-285488	2
Fagron	Tartaric acid	13I25-b01-294093	1
Fagron	Tartaric acid	13I25-B01-294093	3
Fagron	Tartaric acid	13I25-B01-294094	5
Fagron	Tartaric acid	13I25-B01-294095	1
Fagron	Tartaric acid	13l25-B01-285488	1
Fagron	Tartaric acid	14186212	1
Fagron	Tartaric acid	14519	1
Fagron	Tartaric acid	14G07-802	1
Fagron	Tartaric acid	14G07-B02	3
Fagron	Tartaric acid	14G07-B02-308554	3
Fagron	Tartaric acid	14G07-B02-308555	2
Fagron	Tartaric acid	14G07-B02-322976	2
Fagron	Tartaric acid	14G07-B02-322977	1
Fagron	Tartaric acid	14G07-B02-330640	4
Fagron	Tartaric acid	15045303	1
Fagron	Tartaric acid	18G17-B01-351824	1
Fagron	Tartaric acid	20151112-2	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Tartaric acid	20A17-B04-196364	1
Fagron	Tartaric acid	20A17-B04-200531	1
Fagron	Tartaric acid	20A17-B04-200532	2
Fagron	Tartaric acid	20J05-B01-202753	1
Fagron	Tartaric acid	2414E1053	1
Fagron	Tartaric acid	2513M01053	1
Fagron	Tartaric acid	B04-2005302	1
Fagron	Tartaric acid	P161019AT09/18	1
Fagron	Tartaric acid	xxxxxxx	1
fischar, Gehe	Tartaric acid	700061	1
Fischar/Gehe	Tartaric acid	705061	1
Fischar/PH	Tartaric acid	700061	1
Fischar/Phönix 05.07...	Tartaric acid	700061	1
Fischar/Phönix	Tartaric acid	704021	1
Fischar	Tartaric acid	704061	2
Fischar	Tartaric acid	705061	1
Fischar	Tartaric acid	709041	1
Fischer/AHD	Tartaric acid	700061	1
Fragon/Sanacorp	Tartaric acid	13G03-N14	2
Gatt-Koller / Phoenix	Tartaric acid	3334/08131514	1
GEHE 07.05.2014	Tartaric acid	13G03-N14	2
GEHE 14.04.2014	Tartaric acid	12H02-N07	1
Gehe/Fischer	Tartaric acid	706061	1
Gehe/Henry Lamotte	Tartaric acid	17/12	1
Gehe	Tartaric acid	1325-B01-285487	1
Gehe	Tartaric acid	16146806	1
Gehe	Tartaric acid	191825002	2
Gehe	Tartaric acid	21000938008	1
Gehe	Tartaric acid	703061	1
Gehe	Tartaric acid	7284696	1
Hänseler	Tartaric acid		1
Klenk	Tartaric acid	13405	1
L12	Tartaric acid	14G07-B02-308555	1
Nachprüfung	Tartaric acid	2082019-13	1
Noweda 20.7.19	Tartaric acid	18121212	1
Noweda/ Fischar	Tartaric acid	702061	1
Noweda	Tartaric acid	7284696	1
Otto Fischar/ Gehe	Tartaric acid	709041	1
Otto Fischar	Tartaric acid	705061	2
Otto Fischer GmbH	Tartaric acid	705061	1
Phoenix	Tartaric acid	12044115	1
Phoenix	Tartaric acid	12Ho2-N07	1
Phoenix	Tartaric acid	12K29B01	1
Phoenix	Tartaric acid	13116308	1
Phönix Gotha	Tartaric acid	704021	1
Phönix	Tartaric acid	11e24-n06	1
Phönix	Tartaric acid	12286904	1
Phönix	Tartaric acid	13/25-B01-294094	1
Phönix	Tartaric acid	18121208	1
Sanacorp WE: 19.0518...	Tartaric acid	16260406	1
Sanacorp	Tartaric acid	17347104	2
Sanacorp	Tartaric acid	191825005	2
Sanacorp	Tartaric acid	21000301006	1
Sanacorp	Tartaric acid	23000312004	1
schubert / Phoenix	Tartaric acid	1014PLV-755	1
Spangropharm	Tartaric acid	10073111	1

- 235 627 spectra from 1515 *Apo-Ident* customers from a total of 49 081 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are docu-

mented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tartaric acid* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tartaric acid* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	510	0	152 452
Type B	0	190	0	201 894
Type C	0	440	0	235 627

The substance/substance group *Tartaric acid* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8235 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 98.6364 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22383	22613	8.64	218.33
22384	22384	0.00	215.47
22391	22391	0.00	218.71
22501	22391	3.76	220.33
22613	22613	0.00	221.02
24806	24806	0.00	217.46
25628	25628	0.00	222.78
25699	25699	0.00	222.49
26397	22391	5.41	222.57
27307	27307	0.00	227.30

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Taurine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20403-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Taurine; Taurinum

Special notes

When selecting the *Taurine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Taurine	9	5	14

Second-stage model

For differentiation of the substance/substance group *Taurine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Taurine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Menthol	125.73	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Taurine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Taurine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Taurine	1306024-01	21108	50	20130822
Euro OTC	Taurine	1504032-01	21893	60	20150430
Euro OTC	Taurine	1504032-01	21992	60	9167
Euro OTC	Taurine	1602011	22370	60	20160218*
Euro OTC	Taurine	1607035	22795	40	20160819*
Euro OTC	Taurine	1704001	23177	40	20170426*
Euro OTC	Taurine	1904003	24632	40	20190425*
Euro OTC	Taurine	2004002	25406	40	20200615*
Euro OTC	Taurine	2206003	26222	40	20220629*
Euro OTC	Taurine	2206003	26222SI	20	20220629*
Euro OTC	Taurine	2301048	26749	40	20230511*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 490 spectra of 11 reference samples from the substance/substance group *Taurine*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 472 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 7 reference samples from the substance/substance group *Taurine*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Taurine	1711006	23739	40
Euro OTC	Taurine	1810006	24310	40
Euro OTC	Taurine	1910017	24977	40
Euro OTC	Taurine	2309005	26927	40
Euro OTC	Taurine	2310009	26991	40
Euro OTC	Taurine	2301048	26749SI†	20
Euro OTC	Taurine	2309005	26927SI	20

- 201 844 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 31 spectra from 10 *Apo-Ident* customers from 14 batches from the substance/substance group *Taurine*.

- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
Caelo	Taurine	1704001-01	2
el compra import	Taurine	1609025	1
elcompra	Taurine	xp17013244	1
Euro OTC	Taurine	1704001-01	1
Euro OTC	Taurine	1904003-01	1
Euro OTC	Taurine	1910017-01	1
Euro OTC	Taurine	2004002-01	7
Euro OTC	Taurine	2008013-01	6
Euro OTC	Taurine	2008013-02	2
Euro OTC	Taurine	2008013-03	1
Euro OTC	Taurine	2206003-01	4
Euro OTC	Taurine	2301048-01	1
Euro OTC	Taurine	XP16023196	1
Gall Pharma / Phoenix	Taurine		1
hannes	Taurine	1202125	1

- 236 036 spectra from 1515 *Apo-Ident* customers from a total of 49 244 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Taurine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Taurine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	490	0	152 472
Type B	0	240	0	201 844
Type C	0	31	0	236 036

The substance/substance group *Taurine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7755 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 80.6452 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21108	22370	4.14	121.69
21893	22370	3.89	121.09
21992	21992	0.00	121.56
22370	22370	0.00	120.93
22795	22795	0.00	121.56
23177	23177	0.00	120.81
24632	24632	0.00	121.17
25406	25406	0.00	122.23
26222	26222	0.00	121.23
26749	26749	0.00	121.83

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Testosterone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20961-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Testosterone; Testosteronum

Special notes

When selecting the *Testosterone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Testosterone	14	20	114

Second-stage model

For differentiation of the substance/substance group *Testosterone* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Testosterone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prasterone	68.82	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Testosterone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Testosterone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Testosterone	13406004	21370	50	20131219
Caelo	Testosterone	13406004	21371	50	20131219
Caelo	Testosterone	15244906	21987	60	20150814
Caelo	Testosterone	15244906	21987SI	38	20150814
Caelo	Testosterone	16311506	23244	40	20161123
Euro OTC	Testosterone	1307001-01	20961	40	1402309
Euro OTC	Testosterone	1511005	22232	60	20151119*
Euro OTC	Testosterone	1511005	22232SI	35	20151119*
Euro OTC	Testosterone	1604049	22561	40	20160510*
Euro OTC	Testosterone	1604049	22561SI	34	20160510*
Euro OTC	Testosterone	1910001	24963	40	20191024*
Euro OTC	Testosterone	1912017	25104	40	20191216*
Euro OTC	Testosterone	2005006	25160	40	20200519*
Euro OTC	Testosterone	2005006	25160SI	27	20200519*
Euro OTC	Testosterone	2403002	27212	40	20240502*
Fagron	Testosterone	12F13-N02	20729	40	20120628
Fagron	Testosterone	15E18-B08-307772	21970	60	20150526
Fagron	Testosterone	15E18-B08-307772	21970SI	54	20150526
Fagron	Testosterone	17J26-B01-342032	23764	40	20171205
Fagron	Testosterone	22H08-B02-222389	26392	40	20220905
Fagron	Testosterone	22H08-B02-222389	26392SI	40	20220905

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 908 spectra of 21 reference samples from the substance/substance group *Testosterone*. These samples are listed above in the *calibration samples* section. The reference samples come from 14 different batches.
- 152 054 spectra from a total of 2828 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1815 spectra of 47 reference samples from the substance/substance group *Testosterone*.
- Among them are spectra of independent samples from 20 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Testosterone	171199	23347	40
Caelo	Testosterone	181478	24265	40
Caelo	Testosterone	191113	24520	40
Caelo	Testosterone	21002048	25794	40
Euro OTC	Testosterone	1511005-01	21994	60
Euro OTC	Testosterone	1607013	22707	40
Euro OTC	Testosterone	1702017	23146	40
Euro OTC	Testosterone	1802015	23948	40
Euro OTC	Testosterone	1805006	24131	40
Euro OTC	Testosterone	1805021	24132	40
Euro OTC	Testosterone	1808033	24201	40
Euro OTC	Testosterone	1811027	24422	40
Euro OTC	Testosterone	1912014	24964	40
Euro OTC	Testosterone	2008038	25308	40
Euro OTC	Testosterone	2008032	25327	40
Euro OTC	Testosterone	2106009	25705	50
Euro OTC	Testosterone	2110010	25877	50

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Testosterone	2206013	26215	40
Euro OTC	Testosterone	2311029	27004	40
Euro OTC	Testosterone	2407002	27341	40
Caelo	Testosterone	16311506	23244SI†	30
Caelo	Testosterone	171199	23347SI	28
Caelo	Testosterone	171199	23670	40
Caelo	Testosterone	171199	23670SI	30
Caelo	Testosterone	181478	24265SI	40
Caelo	Testosterone	191113	24520SI	40
Caelo	Testosterone	21002048	25794SI	40
Euro OTC	Testosterone	1511005-01	21994SI	32
Euro OTC	Testosterone	1607013	22707SI	40
Euro OTC	Testosterone	1702017	23146SI	21
Euro OTC	Testosterone	1802015	23948SI	40
Euro OTC	Testosterone	1805006	24131SI	40
Euro OTC	Testosterone	1805021	24132SI	40
Euro OTC	Testosterone	1808033	24201SI	40
Euro OTC	Testosterone	1811027	24422SI	26
Euro OTC	Testosterone	1910001	24963SI†	39
Euro OTC	Testosterone	1912014	24964SI	30
Euro OTC	Testosterone	1912017	25104SI†	40
Euro OTC	Testosterone	2008038	25308SI	36
Euro OTC	Testosterone	2008032	25327SI	40
Euro OTC	Testosterone	2106009	25705SI	49
Euro OTC	Testosterone	2110010	25877SI	50
Euro OTC	Testosterone	2206013	26215SI	40
Euro OTC	Testosterone	2311029	27004SI	32
Euro OTC	Testosterone	2403002	27212SI†	30
Euro OTC	Testosterone	2407002	27341SI	32
Fagron	Testosterone	17J26-B01-342032	23764SI†	30

- 200 269 spectra from a total of 4020 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 369 spectra from 111 *Apo-Ident* customers from 122 batches from the substance/substance group *Testosterone*.

- Among them are spectra of independent samples from 114 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Testosterone	2206013-02	4
	Testosterone	23000429008	1
	Testosterone	2311029-01	1
	Testosterone	23K14-B10230723	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Testosterone	23K14-B10-230723	1
	Testosterone	2403002	1
Audor Pharma	Testosterone	AP5106061T	5
Audor Pharma	Testosterone	APZTST16001-M1T	1
Audor Pharma	Testosterone	APZTSTG18003T	10
Audor Pharma	Testosterone	apztstg18004t	2
Audor Pharma	Testosterone	APZTSTG18004T	3
Caelo	Testosterone		1
Caelo	Testosterone	11/07-N12	1
Caelo	Testosterone	12176301	1
Caelo	Testosterone	12176305	3
Caelo	Testosterone	13134804	1
Caelo	Testosterone	13134806	4
Caelo	Testosterone	13134808	1
Caelo	Testosterone	13406004	2
Caelo	Testosterone	14201105	1
Caelo	Testosterone	14355605	1
Caelo	Testosterone	15195802	1
Caelo	Testosterone	15195803	1
Caelo	Testosterone	15244906	1
Caelo	Testosterone	15412201	5
Caelo	Testosterone	15412202	3
Caelo	Testosterone	1604049-01	1
Caelo	Testosterone	16225804	3
Caelo	Testosterone	16225807	2
Caelo	Testosterone	16311506	1
Caelo	Testosterone	17119902	2
Caelo	Testosterone	17119903	1
Caelo	Testosterone	17119911	1
Caelo	Testosterone	1805021-01	2
Caelo	Testosterone	1811027-01	1
Caelo	Testosterone	18147803	7
Caelo	Testosterone	18147810	1
Caelo	Testosterone	19111302	1
Caelo	Testosterone	192738003	1
Caelo	Testosterone	192738006	5
Caelo	Testosterone	192738009	1
Caelo	Testosterone	19273803	2
Caelo	Testosterone	20004205001	1
Caelo	Testosterone	20004205002	1
Caelo	Testosterone	20004205004	1
Caelo	Testosterone	21002048002	2
Caelo	Testosterone	21002048003	1
Caelo	Testosterone	21002048004	2
Caelo	Testosterone	21002048009	7
Caelo	Testosterone	21002048010	1
Caelo	Testosterone	AP5106061T	1
Caelo	Testosterone	APL00034466T	1
Caelo	Testosterone	APZTSTG18004T	1
Caesar & Loretz GmbH...	Testosterone	21002048002	1
Caesar & Loretz GmbH	Testosterone	18147803	1
Caesar & Loretz GmbH	Testosterone	19273804	2
Caesar & Loretz GmbH	Testosterone	20004205002	1
Caesar & Loretz GmbH	Testosterone	20004205007	1
Caesar & Loretz GmbH	Testosterone	21002048002	1
erou	Testosterone	2110010-02	1
EuRho	Testosterone	1811027	1
Euro OTC	Testosterone	1106011-01	1
Euro OTC	Testosterone	1106011-03	4
Euro OTC	Testosterone	11o6011-03	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Testosterone	1207005-02	1
Euro OTC	Testosterone	130700101	1
Euro OTC	Testosterone	1307001-01	5
Euro OTC	Testosterone	140400201	1
Euro OTC	Testosterone	1404002-01	3
Euro OTC	Testosterone	1404002-1	1
Euro OTC	Testosterone	1511005-01	6
Euro OTC	Testosterone	1604049-01	17
Euro OTC	Testosterone	1607013-01	1
Euro OTC	Testosterone	1607013-02	9
Euro OTC	Testosterone	1702017-01	41
Euro OTC	Testosterone	1802015	1
Euro OTC	Testosterone	180500601	1
Euro OTC	Testosterone	1805006-01	1
Euro OTC	Testosterone	1805021-01	9
Euro OTC	Testosterone	180506-01	1
Euro OTC	Testosterone	1808033-01	3
Euro OTC	Testosterone	1811027	1
Euro OTC	Testosterone	1811027-01	10
Euro OTC	Testosterone	1811027-02	1
Euro OTC	Testosterone	18147813	2
Euro OTC	Testosterone	1910001-01	5
Euro OTC	Testosterone	1912014-01	5
Euro OTC	Testosterone	1912017-01	1
Euro OTC	Testosterone	2005006-01	2
Euro OTC	Testosterone	2008032-01	10
Euro OTC	Testosterone	2008038-01	14
Euro OTC	Testosterone	2008038-02	1
Euro OTC	Testosterone	2106009-01	9
Euro OTC	Testosterone	2106009-02	4
Euro OTC	Testosterone	2110010-01	7
Euro OTC	Testosterone	2110010-02	1
Euro OTC	Testosterone	2403002-01	1
Euro OTC	Testosterone	3x1106011-03	1
Euro OTC	Testosterone	APZTSTG18003T	1
Euro OTC	Testosterone	ZTSTy18004	1
Euro TOC	Testosterone	1811027-02	1
EUro/AHD	Testosterone	1106011-03	1
Euroo/Phoenix	Testosterone	1307001-01	1
Fagron	Testosterone	11/07-N12	1
Fagron	Testosterone	12F13-N02	1
Fagron	Testosterone	13g10n03	1
Fagron	Testosterone	13G10-N03	2
Fagron	Testosterone	13I26-N08	1
Fagron	Testosterone	13L09-B03-294148	1
Fagron	Testosterone	13l09b03294149	1
Fagron	Testosterone	13l09b03298118	1
Fagron	Testosterone	15E18-B08	1
Fagron	Testosterone	16A20-B11-318899	7
Fagron	Testosterone	1712-B05	1
Fagron	Testosterone	17A12-B05-331496	1
Fagron	Testosterone	17J26-B01-342033	2
Fagron	Testosterone	17J26-B01-342637	4
Fagron	Testosterone	18A25-B03-350800	2
Fagron	Testosterone	19B12-B01	5
Fagron	Testosterone	19J04-F04_365938	1
Fagron	Testosterone	19J04-F04-365936	1
Fagron	Testosterone	20804-F03-370229	3
Fagron	Testosterone	20B04-F03	1
Fagron	Testosterone	23K14-B10-233057	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Testosterone	24B26-B07-237509	1
Fagron	Testosterone	F03-3702209	1
Fagron	Testosterone	GTJ151103	1
Gatt-Koller	Testosterone	22J00592	1
Gehe	Testosterone	1805021-01	1
Gehe	Testosterone	1811027-01	3
GEHE	Testosterone	1912014-01	1
Geilenkirchen	Testosterone	16225803	1
Haihang Industry	Testosterone	20140114-1	1
Haihang Industry	Testosterone	20140114-2	1
Hubei Zhuxi Humanwell	Testosterone	2005006-01	1
Noweda	Testosterone	1702017-01	1
Noweda	Testosterone	19111303	1
Noweda	Testosterone	23000429008	1
Noweda	Testosterone	2311029-01	1
NWM CHina	Testosterone	TE150402	1
Pharbil Waltrop GmbH	Testosterone	9542100/228178-0	1
Phönix Gotha	Testosterone	1106011-03	1
Phönix Gotha	Testosterone	1408015-01	1
Sanacorp	Testosterone	2110010-01	1
Sanacorp	Testosterone	23000429006	1
Shandong Northwest M…	Testosterone	GTJ160510	1
Spirig	Testosterone	13406003	1

- 235 698 spectra from 1515 *Apo-Ident* customers from a total of 49 139 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Testosterone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Testosterone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	908	0	152 054
Type B	0	1815	0	200 269
Type C	0	363	6	235 698

The substance/substance group *Testosterone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.3392 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.6694 %)
Type C	100.0000 % (> 99.9007 %)	98.3740 % (> 97.5610 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20729	24963	14.17	132.21
20961	20961	0.00	133.50
21370	22232	7.73	132.27
21371	22232	8.86	132.66
21970	22232	4.10	132.32
21987	22232	3.35	133.14
22232	22232	0.00	133.44
22561	22561	0.00	125.49
23244	22232	6.22	133.39
23764	22232	6.35	133.95
24963	24963	0.00	132.78
25104	25104	0.00	136.17
25160	25160	0.00	131.72
26392	25104	15.02	134.91
27212	27212	0.00	135.19

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Testosterone propionate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20880-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Testosterone propionate; Testosteroni propionas

Special notes

When selecting the *Testosterone propionate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Testosterone propionate	6	11	278

Second-stage model

For differentiation of the substance/substance group *Testosterone propionate* the following second-stage model is used:

- Submodel 05

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Testosterone propionate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Progesterone	37.34	48.82
Spironolactone	49.58	49.67
⋮	⋮	⋮
Povidone iodine	>50	84.15
Povidone	>50	84.83
Fusidic acid	>50	114.35
Ubidecarenone	>50	127.06

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Testosterone propionate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Testosterone propionate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Testosterone propionate	12163607	20880	40	AR-15-FG-000623-01
Caelo	Testosterone propionate	15444709	23170	40	1707612
Euro OTC	Testosterone propionate	1109024-02	21644	60	1503607
Euro OTC	Testosterone propionate	1511003	22230	60	20151111*
Euro OTC	Testosterone propionate	1511003	22230SI	43	20151111*
Euro OTC	Testosterone propionate	1512023	22288	45	20151230*
Euro OTC	Testosterone propionate	1512023	22288SI	45	20151230*
Euro OTC	Testosterone propionate	2003011	25116	40	20200408*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 373 spectra of 8 reference samples from the substance/substance group *Testosterone propionate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 589 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 939 spectra of 24 reference samples from the substance/substance group *Testosterone propionate*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Testosterone propionate	170963	23334	40
Caelo	Testosterone propionate	191986	24759	40
Caelo	Testosterone propionate	22003581	26494	40
Caelo	Testosterone propionate	23001951	26952	40
Euro OTC	Testosterone propionate	1710027	23734	40
Euro OTC	Testosterone propionate	1811040	24413	40
Euro OTC	Testosterone propionate	2010004	25476	40
Euro OTC	Testosterone propionate	2206019	26205	40
Euro OTC	Testosterone propionate	2309024	26925	40
Fagron	Testosterone propionate	22F07-F03-382822	26373	40
Fagron	Testosterone propionate	24E02-B03-241020	27411	40
Caelo	Testosterone propionate	15444709	23170SI†	30
Caelo	Testosterone propionate	170963	23334SI	29
Caelo	Testosterone propionate	191986	24759SI	40
Caelo	Testosterone propionate	22003581	26494SI	40
Caelo	Testosterone propionate	23001951	26952SI	40
Euro OTC	Testosterone propionate	1710027	23734SI	40
Euro OTC	Testosterone propionate	1811040	24413SI	40
Euro OTC	Testosterone propionate	2003011	25116SI†	40
Euro OTC	Testosterone propionate	2010004	25476SI	40
Euro OTC	Testosterone propionate	2206019	26205SI	40
Euro OTC	Testosterone propionate	2309024	26925SI	40
Fagron	Testosterone propionate	22F07-F03-382822	26373SI	40
Fagron	Testosterone propionate	24E02-B03-241020	27411SI	40

- 201 145 spectra from a total of 4032 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 934 spectra from 428 *Apo-Ident* customers from 294 batches from the substance/substance group *Testosterone propionate*.

- Among them are spectra of independent samples from 278 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Testosterone propionate	16C24-B04-320784	2
	Testosterone propionate	2010004-02	1
	Testosterone propionate	2206019-01	1
	Testosterone propionate	2206019-02	4
	Testosterone propionate	22K07-B09	1
	Testosterone propionate	22K07-B09-223645	2
	Testosterone propionate	22K07-b09-223647	1
	Testosterone propionate	22K07-B09-223647	6
	Testosterone propionate	22K07-B09-228637	7
	Testosterone propionate	23J09-B10-233051	2
	Testosterone propionate	f03-3828201	1
	Testosterone propionate	TSP103/0322	2
AHD	Testosterone propionate	17325712	1
AHD	Testosterone propionate	19K11-F05	1
AHD	Testosterone propionate	AP12E04-N01TP	1
AHL	Testosterone propionate	APZTSP15003-MTP	2
Alliance	Testosterone propionate	2206019-02	1
Alliance	Testosterone propionate	22k07-b09-223645	1
allianz	Testosterone propionate	15444704	1
Andor	Testosterone propionate	1109024-03TP	1
Anzag	Testosterone propionate	14L31-B02-304722	1
Anzag	Testosterone propionate	20K26-F06-375792	1
Apo-ident / AH	Testosterone propionate	2003011-01	1
apomix	Testosterone propionate	13K25-B05-287648	1
apomix	Testosterone propionate	40/14	1
Audor Pharma	Testosterone propionate	AP1109024-03	2
Audor Pharma	Testosterone propionate	AP1109024-03TP	4
Audor Pharma	Testosterone propionate	AP12E04N01TP	2
Audor Pharma	Testosterone propionate	AP12J10-N08TP	2
Audor Pharma	Testosterone propionate	AP13K25-B05-287643T	1
Audor Pharma	Testosterone propionate	AP13K25-B05-287643TP	1
Audor Pharma	Testosterone propionate	APZTSP15003-MTP	16
Audor Pharma	Testosterone propionate	APZTSP1503-MTP	1
Caelo	Testosterone propionate	10235809	1
Caelo	Testosterone propionate	103004	1
Caelo	Testosterone propionate	106212376	1
Caelo	Testosterone propionate	1108212376	1
Caelo	Testosterone propionate	1109024-02	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Testosterone propionate	12060102	2
Caelo	Testosterone propionate	12163605	2
Caelo	Testosterone propionate	12163607	1
Caelo	Testosterone propionate	12163610	2
Caelo	Testosterone propionate	12163612	6
Caelo	Testosterone propionate	12163613	1
Caelo	Testosterone propionate	12163615	2
Caelo	Testosterone propionate	12163616	4
Caelo	Testosterone propionate	12163617	4
Caelo	Testosterone propionate	12163619	2
Caelo	Testosterone propionate	12163621	1
Caelo	Testosterone propionate	1263607	1
Caelo	Testosterone propionate	12A02-N05	1
Caelo	Testosterone propionate	12J10-N08	2
Caelo	Testosterone propionate	13C08-N02	1
Caelo	Testosterone propionate	13F05-N04	1
Caelo	Testosterone propionate	13K25-B05-291974	1
Caelo	Testosterone propionate	14D15-B03-296959	1
Caelo	Testosterone propionate	14L31-B02-304722	2
Caelo	Testosterone propionate	15003002	8
Caelo	Testosterone propionate	15003004	3
Caelo	Testosterone propionate	15003008	2
Caelo	Testosterone propionate	151100301	1
Caelo	Testosterone propionate	1511003-01	1
Caelo	Testosterone propionate	15169504	1
Caelo	Testosterone propionate	15444702	10
Caelo	Testosterone propionate	15444703	16
Caelo	Testosterone propionate	15444705	4
Caelo	Testosterone propionate	15444706	3
Caelo	Testosterone propionate	15444707	4
Caelo	Testosterone propionate	15444709	1
Caelo	Testosterone propionate	15444710	5
Caelo	Testosterone propionate	15444711	1
Caelo	Testosterone propionate	15444712	1
Caelo	Testosterone propionate	15444713	2
Caelo	Testosterone propionate	15444714	3
Caelo	Testosterone propionate	15444717	1
Caelo	Testosterone propionate	15444718	2
Caelo	Testosterone propionate	15444719	1
Caelo	Testosterone propionate	15444721	2
Caelo	Testosterone propionate	15444723	1
Caelo	Testosterone propionate	1544717	1
Caelo	Testosterone propionate	16E24-B01-324711	2
Caelo	Testosterone propionate	16H22-B05-326483	1
Caelo	Testosterone propionate	1710027-01	2
Caelo	Testosterone propionate	17325707	10
Caelo	Testosterone propionate	17325709	2
Caelo	Testosterone propionate	17325711	2
Caelo	Testosterone propionate	17325712	2
Caelo	Testosterone propionate	17325712P-190312-8	1
Caelo	Testosterone propionate	17325716	1
Caelo	Testosterone propionate	17325717	9
Caelo	Testosterone propionate	17325719	2
Caelo	Testosterone propionate	17B09B03332376	1
Caelo	Testosterone propionate	17B09-B03-332376	1
Caelo	Testosterone propionate	17J16-B03-341320	1
Caelo	Testosterone propionate	18b06-B04	1
Caelo	Testosterone propionate	18b06-b04-351510	1
Caelo	Testosterone propionate	18B14-B02-353456	1
Caelo	Testosterone propionate	18I12-B03-355137	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Testosterone propionate	191986001	3
Caelo	Testosterone propionate	191986003	1
Caelo	Testosterone propionate	191986007	2
Caelo	Testosterone propionate	19198603	6
Caelo	Testosterone propionate	19198603P-200319-13	1
Caelo	Testosterone propionate	19198604	8
Caelo	Testosterone propionate	19k11-f05-366325	1
Caelo	Testosterone propionate	2013U-02376	1
Caelo	Testosterone propionate	20H19-F07-373643	1
Caelo	Testosterone propionate	21000430001	1
Caelo	Testosterone propionate	21000430002	3
Caelo	Testosterone propionate	21000430006	2
Caelo	Testosterone propionate	21000430010	1
Caelo	Testosterone propionate	22003581002	3
Caelo	Testosterone propionate	22K07-B09-223647	1
Caelo	Testosterone propionate	23051816	1
Caelo	Testosterone propionate	2910030-02	1
Caelo	Testosterone propionate	36814m1	1
Caelo	Testosterone propionate	36814M1	2
Caelo	Testosterone propionate	612212376	1
Caelo	Testosterone propionate	614E2376	1
Caelo	Testosterone propionate	903312376	1
Caesar & Loretz GmbH...	Testosterone propionate	17325719	1
Caesar & Loretz GmbH...	Testosterone propionate	19198603	1
Caesar & Loretz GmbH...	Testosterone propionate	21000430006	2
Caesar & Loretz GmbH...	Testosterone propionate	17325722	1
Caesar & Loretz GmbH...	Testosterone propionate	19198604	2
Caesar & Loretz GmbH	Testosterone propionate	17325716	1
Caesar & Loretz GmbH	Testosterone propionate	17325717	2
CAESAR & LORETZ GMBH	Testosterone propionate	191986003	2
Caesar & Loretz GmbH	Testosterone propionate	191986006	1
Caesar & Loretz GmbH	Testosterone propionate	19198603	2
Caesar & Loretz GmbH	Testosterone propionate	19198604	5
Caesar & Loretz GmbH	Testosterone propionate	21000430002	1
Caesar & Loretz GmbH	Testosterone propionate	21000430006	1
Caesar & Loretz GmbH	Testosterone propionate	21000430009	3
Caesar & Loretz GmbH	Testosterone propionate	21000430010	1
Caesar & Loretz GmbH	Testosterone propionate	21000430012	2
Caesar & Loretz GmbH	Testosterone propionate	22003581003	1
Ebert 17.08.16	Testosterone propionate	15444703	1
EURHO/Anzag	Testosterone propionate	1811040-01	1
EuRho/Krieger	Testosterone propionate	1811040-01	3
EuRho	Testosterone propionate	17100271	1
EuRho	Testosterone propionate	1811040-01	1
EuRho	Testosterone propionate	2003011-01	1
Euro OTC	Testosterone propionate	101/0218	1
Euro OTC	Testosterone propionate	1103010-01	1
Euro OTC	Testosterone propionate	1103010-02	1
Euro OTC	Testosterone propionate	1109024-02	1
Euro OTC	Testosterone propionate	1109024-03	1
Euro OTC	Testosterone propionate	1409037-01	2
Euro OTC	Testosterone propionate	1504023-01	5
Euro OTC	Testosterone propionate	1511003-01	10
Euro OTC	Testosterone propionate	1512023-01	2
Euro OTC	Testosterone propionate	15444718	2
Euro OTC	Testosterone propionate	1710027-01	8
Euro OTC	Testosterone propionate	181040-01	1
Euro OTC	Testosterone propionate	181104001	2
Euro OTC	Testosterone propionate	1811040-01	16
Euro OTC	Testosterone propionate	18111709	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Testosterone propionate	18114001	1
Euro OTC	Testosterone propionate	2003011-01	10
Euro OTC	Testosterone propionate	2010004-01	14
Euro OTC	Testosterone propionate	2010004-02	1
Euro OTC	Testosterone propionate	710027-01	1
Euro OTC	Testosterone propionate	970116/1	1
Euro OTC	Testosterone propionate	F07-3736403	1
Euro/Lui	Testosterone propionate	1811040-01	1
euro	Testosterone propionate	2010004-01	1
Fagro/Noweda	Testosterone propionate	16H22-B05-326483	2
Fagron	Testosterone propionate		2
Fagron	Testosterone propionate	10L03-N16	3
Fagron	Testosterone propionate	11/12-N03	1
Fagron	Testosterone propionate	11C21-N09	1
Fagron	Testosterone propionate	11G15-N07	3
Fagron	Testosterone propionate	11K18-N04	4
Fagron	Testosterone propionate	12/10-N08	1
Fagron	Testosterone propionate	12163616	2
Fagron	Testosterone propionate	12A02-N05	2
Fagron	Testosterone propionate	12C01-N01	1
Fagron	Testosterone propionate	12C01-NO1	1
Fagron	Testosterone propionate	12E04-N01	3
Fagron	Testosterone propionate	12E29-N02	1
Fagron	Testosterone propionate	12J10N-08	1
Fagron	Testosterone propionate	12J10-N08	4
Fagron	Testosterone propionate	13/03-N02	2
Fagron	Testosterone propionate	13C08N02	1
Fagron	Testosterone propionate	13C08-N02	15
Fagron	Testosterone propionate	13F05-N04	16
Fagron	Testosterone propionate	13I03-N02	1
Fagron	Testosterone propionate	13K25-B05	1
Fagron	Testosterone propionate	13K25-B05-287647	10
Fagron	Testosterone propionate	13K25B05287648	1
Fagron	Testosterone propionate	13K25-B05-287648	5
Fagron	Testosterone propionate	13K25-B05-291974	2
Fagron	Testosterone propionate	14A28-B12	2
Fagron	Testosterone propionate	14A28-B12-291977	1
Fagron	Testosterone propionate	14A28B12296958	1
Fagron	Testosterone propionate	14A28-B12-296958	2
Fagron	Testosterone propionate	14A28-B12-296960	2
Fagron	Testosterone propionate	14D15-B03-296959	4
Fagron	Testosterone propionate	14l31-B02	1
Fagron	Testosterone propionate	14L31-B02	4
Fagron	Testosterone propionate	14L31B02-304721	1
Fagron	Testosterone propionate	14L31-B02-304721	9
Fagron	Testosterone propionate	14L31B02304722	1
Fagron	Testosterone propionate	14L31-B02-304722	11
Fagron	Testosterone propionate	15/01-B09	1
Fagron	Testosterone propionate	15/01-B09-312867	1
Fagron	Testosterone propionate	15/01-B09-318371	2
Fagron	Testosterone propionate	1501-B09-312867	1
Fagron	Testosterone propionate	1511003-01	1
Fagron	Testosterone propionate	15444717	1
Fagron	Testosterone propionate	15D03-B02-310694	1
Fagron	Testosterone propionate	15I01-B01-318371	1
Fagron	Testosterone propionate	15I01-B09-312867	2
Fagron	Testosterone propionate	15I01-B09-318371	2
Fagron	Testosterone propionate	15k03-b03	1
Fagron	Testosterone propionate	15K03-B03-315218	7
Fagron	Testosterone propionate	15K03-B-03-315218	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Testosterone propionate	15l01-B09-312867	1
Fagron	Testosterone propionate	16C24B04320784	1
Fagron	Testosterone propionate	16C24-B04-320784	4
Fagron	Testosterone propionate	16E24-B01	1
Fagron	Testosterone propionate	16E24-B01-322593	7
Fagron	Testosterone propionate	16E24B01322938	1
Fagron	Testosterone propionate	16E24B01324711	1
Fagron	Testosterone propionate	16E24-B01-324711	2
Fagron	Testosterone propionate	16E24-B01-325476	1
Fagron	Testosterone propionate	16E24-Bo1-322938	1
Fagron	Testosterone propionate	16H22-B05	2
Fagron	Testosterone propionate	16H22-B05-326482	4
Fagron	Testosterone propionate	16h22-b05-326483	1
Fagron	Testosterone propionate	16H22B05326483	1
Fagron	Testosterone propionate	16H22-B05-326483	12
Fagron	Testosterone propionate	16K24B03330544	1
Fagron	Testosterone propionate	16K24-B03-330544	1
Fagron	Testosterone propionate	17116-B04-346529	1
Fagron	Testosterone propionate	17B09-B03	1
Fagron	Testosterone propionate	17B09B03332376	1
Fagron	Testosterone propionate	17B09-B03-332376	6
Fagron	Testosterone propionate	17B09-B04-335269	2
Fagron	Testosterone propionate	17E22-B09	1
Fagron	Testosterone propionate	17E22-B09-338592	4
Fagron	Testosterone propionate	17H25-B02-341321	4
Fagron	Testosterone propionate	17J16-B03	1
Fagron	Testosterone propionate	17j16-B03-341320	1
Fagron	Testosterone propionate	17J16B03-341320	2
Fagron	Testosterone propionate	17J16-B03-341320	1
Fagron	Testosterone propionate	17J16-B03-343010	4
Fagron	Testosterone propionate	17J16-B03-344243	2
Fagron	Testosterone propionate	17J16B04346529	1
Fagron	Testosterone propionate	17J16-B04-346529	7
Fagron	Testosterone propionate	18/12-B03	1
Fagron	Testosterone propionate	18/12-B03-355296	2
Fagron	Testosterone propionate	18/12-B03-3567	1
Fagron	Testosterone propionate	18/12-B03-356702	4
Fagron	Testosterone propionate	18/12-B03-356703	4
Fagron	Testosterone propionate	18/12-B03-3596	1
Fagron	Testosterone propionate	18B06-B04	2
Fagron	Testosterone propionate	18B06-B04-348557	4
Fagron	Testosterone propionate	18B06B04350560	1
Fagron	Testosterone propionate	18B06-B04-350560	1
Fagron	Testosterone propionate	18B06-B04-351510	7
Fagron	Testosterone propionate	18B06-B04-352492	4
Fagron	Testosterone propionate	18B06-B04-352493	6
Fagron	Testosterone propionate	18b14-b02-353456	1
Fagron	Testosterone propionate	18B14-B02-353456	2
Fagron	Testosterone propionate	18I12-B03	1
Fagron	Testosterone propionate	18I12-B03-355137	2
Fagron	Testosterone propionate	18I12-B03-355296	2
Fagron	Testosterone propionate	18I12-B03-356702	1
Fagron	Testosterone propionate	18I12-B03-356703	2
Fagron	Testosterone propionate	18I22-B03-356703	1
Fagron	Testosterone propionate	18l12-B03-356703	1
Fagron	Testosterone propionate	19H16-F03-364849	4
Fagron	Testosterone propionate	19H16-F03-364850	7
Fagron	Testosterone propionate	19H22-B05-326483	1
Fagron	Testosterone propionate	19K11-F05-366324	9
Fagron	Testosterone propionate	19K11-F05-366325	11

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Testosterone propionate	20121012-3	1
Fagron	Testosterone propionate	20A27-F08	2
Fagron	Testosterone propionate	20A27-F08-368802	6
Fagron	Testosterone propionate	20A27-F08-368803	1
Fagron	Testosterone propionate	20A27-F08-368803	2
Fagron	Testosterone propionate	20A27F08369542	1
Fagron	Testosterone propionate	20A27-F08-369542	2
Fagron	Testosterone propionate	20F24-F02	1
Fagron	Testosterone propionate	20F24-F02-371915	7
Fagron	Testosterone propionate	20F24-F02-371916	10
Fagron	Testosterone propionate	20F24-FO2-371915	1
Fagron	Testosterone propionate	20H19-F07	2
Fagron	Testosterone propionate	20H19-F07-3736403	1
Fagron	Testosterone propionate	20H19-F07-373642	6
Fagron	Testosterone propionate	20H19-F07-373643	9
Fagron	Testosterone propionate	20H19-F07-373643	1
Fagron	Testosterone propionate	20H19-F07-375282	4
Fagron	Testosterone propionate	20K26-F06	3
Fagron	Testosterone propionate	20K26-F06-375792	6
Fagron	Testosterone propionate	20K26-F06-375793	7
Fagron	Testosterone propionate	21J04-F03	2
Fagron	Testosterone propionate	21J04F03-380627	1
Fagron	Testosterone propionate	21J04-F03-380627	11
Fagron	Testosterone propionate	21J04-F03-380628	13
Fagron	Testosterone propionate	21JO4-F03-380627	1
Fagron	Testosterone propionate	22F07-03F-382821	1
Fagron	Testosterone propionate	22F07-F03-382821	7
Fagron	Testosterone propionate	22K07-B09	1
Fagron	Testosterone propionate	22K07-B09-223647	1
Fagron	Testosterone propionate	24411M1	1
Fagron	Testosterone propionate	2OF24-FO2-371915	1
Fagron	Testosterone propionate	2OK26-F06-375792	1
Fagron	Testosterone propionate	2OK26-FO6-375792	1
Fagron	Testosterone propionate	32012M1	1
Fagron	Testosterone propionate	3380627	1
Fagron	Testosterone propionate	3613M-02376	1
Fagron	Testosterone propionate	36513M1	3
Fagron	Testosterone propionate	36814M1	2
Fagron	Testosterone propionate	6081201	1
Fagron	Testosterone propionate	APZTSP15003-MTP	2
Fagron	Testosterone propionate	F02-3719105	2
Fagron	Testosterone propionate	F02-3719106	1
Fagron	Testosterone propionate	F03-3648500	1
Fagron	Testosterone propionate	F06-3757902	7
Fagron	Testosterone propionate	F06-3757903	1
Fagron	Testosterone propionate	F07-3736402	2
Fagron	Testosterone propionate	F07-3736403	2
Fagron	Testosterone propionate	F07-3752802	2
Fagron	Testosterone propionate	F08-3688002	1
Fagron	Testosterone propionate	F08-3688003	2
Fagron	Testosterone propionate	T009/07109	2
Fagron	Testosterone propionate	t011/072000	1
Fagron	Testosterone propionate	TSP101/0720	1
Fagron	Testosterone propionate	TSP102/0720	1
Fagron	Testosterone propionate	TSP-BLT008/0719	1
Fagron	Testosterone propionate	TSP-BLT011/0720	1
Fargon - Alliance He...	Testosterone propionate	18/12-B03-356703	1
Fargon /Max Jenne	Testosterone propionate	18I12-B03-355296	1
Fargon/ Phönix	Testosterone propionate	18I12-B03-356703	1
Fargon/Kehr	Testosterone propionate	17B09-B04-335269	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fargon	Testosterone propionate	19K11-F05_366324	1
Fiebig	Testosterone propionate	20F24-F02-371915	1
Fragon	Testosterone propionate	21j04-F03-380628	1
Galderma	Testosterone propionate	15K03-B03-315218	1
Gatt-Koller	Testosterone propionate	1803006	1
Gatt-Koller	Testosterone propionate	3478/09153915	1
Gatt-Koller	Testosterone propionate	606213811	1
Gehe/Euro	Testosterone propionate	1200318/151100301	1
Gehe/Fragon	Testosterone propionate	17B09B03332376	1
Gehe	Testosterone propionate	14A28B12296958	1
Gehe	Testosterone propionate	15444706	1
Gehe	Testosterone propionate	16H22-B05	1
GEHE	Testosterone propionate	17325709	1
GEHE	Testosterone propionate	17325712	1
Gehe	Testosterone propionate	19H16-F03	1
Gehe	Testosterone propionate	19H16-F03-364849	1
Gehe	Testosterone propionate	19K11-F05-366325	1
Gehe	Testosterone propionate	20K26-F06-375792	1
Gehe	Testosterone propionate	22K07-B09-228637	1
Infectopharm/Phönix	Testosterone propionate	18B06-B04-352493	1
Jenne	Testosterone propionate	22003581003	1
Jenne	Testosterone propionate	22K07-B09-228637	1
Kehr/Fargon	Testosterone propionate	17J16-B03-344243	1
Kehr/Fargon	Testosterone propionate	18/12-B03-355296	2
Kehr	Testosterone propionate	2206019-01	1
Noweda	Testosterone propionate	12163610	1
Noweda	Testosterone propionate	1511003	1
Noweda	Testosterone propionate	17B09-B03-332376	1
Noweda	Testosterone propionate	2206019-01	2
Noweda	Testosterone propionate	22F07-F03-382821	1
Noweda	Testosterone propionate	22K07-B09-223647	1
Noweda	Testosterone propionate	22K07-B09-228637	1
Phoenix/Cealo	Testosterone propionate	36814M1	1
Phoenix	Testosterone propionate	1109024-02	1
phoenix	Testosterone propionate	12163615	1
Phönix WE:25.04.16 E...	Testosterone propionate	14L31-B02-304722	1
Phönix/ Fargon	Testosterone propionate	16H22-B05-326483	3
Phönix/ Fargon	Testosterone propionate	19H16-F03-364850	1
Phönix/Euro	Testosterone propionate	110301002	1
Phönix	Testosterone propionate	12163613	1
Phönix	Testosterone propionate	12163617	1
Phönix	Testosterone propionate	12J10-N08	1
Phönix	Testosterone propionate	13C08-N02	1
Phönix	Testosterone propionate	13K25-B05	1
Phönix	Testosterone propionate	14L31-B02-304722	1
Phönix	Testosterone propionate	15444702	1
Phönix	Testosterone propionate	15444707	1
Phönix	Testosterone propionate	15444710	1
PHÖNIX	Testosterone propionate	15444720	1
Phönix	Testosterone propionate	17325704	1
Phönix	Testosterone propionate	20H19-F07-373643	1
Sanacorp 12.06.2019 6,70EUR	Testosterone propionate	1710027-01	1
Sanacorp	Testosterone propionate	13K25-B05	1
Sanacorp	Testosterone propionate	14L31-B02-304721	2
Sanacorp	Testosterone propionate	18B06-B0	1
Sanacorp	Testosterone propionate	18I12-B03	1
Sanacorp	Testosterone propionate	19H16-F03	1
Sanacorp	Testosterone propionate	20A27-F09	1
Sanacorp	Testosterone propionate	21J04-F03	1
Sanacorp	Testosterone propionate	22Fo7-F03-382822	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Testosterone propionate	TSP103/0322	2
symbiotec	Testosterone propionate	APZTSP15003-MTP	1
Symbiotica Speciality	Testosterone propionate	15444702	2

- 235 133 spectra from 1515 *Apo-Ident* customers from a total of 48 966 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Testosterone propionate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Testosterone propionate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	373	0	152 589
Type B	0	939	0	201 145
Type C	0	848	86	235 133

The substance/substance group *Testosterone propionate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3914 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.3610 %)
Type C	100.0000 % (> 99.9007 %)	90.7923 % (> 90.4711 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20880	20880	0.00	39.75
21644	21644	0.00	38.36
22230	22230	0.00	38.89

continued on the next page

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22288	22288	0.00	38.65
23170	23170	0.00	37.34
25116	25116	0.00	41.90

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tetracaine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20947-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tetracaine; Tetracainum

Special notes

When selecting the *Tetracaine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tetracaine	9	13	161

Second-stage model

For differentiation of the substance/substance group *Tetracaine* the following second-stage model is used:

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tetracaine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	152.18	–
⋮	⋮	⋮
Capsaicin	>50	116.99
Prednicarbate	>50	154.01
Cyproterone acetate	>50	189.86
Oxybutynin hydrochloride	>50	197.97
Alfatradiol	>50	223.11
Levocarnitine	>50	226.28
Sodium citrate	>50	241.75
Amitriptyline hydrochloride	>50	252.29
Norethisterone acetate	>50	349.52
Heparin sodium	>50	410.79
Pyridoxal-5-phosphate	>50	500.87
Quinine hydrochloride dihydrate	>50	535.08
Methoxsalen	>50	590.00
Ciprofloxacin hydrochloride	>50	798.53
Valine	>50	1050.21
Amifampridine	>50	1510.72
Triclosan	>50	1768.56
Sucrose	>50	2140.85

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tetracaine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tetracaine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Tetracaine	171117	23321	40	20170512*
Caelo	Tetracaine	181249	24255	40	20180605*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Tetracaine	1405025-01	21603	60	AR-14-FG-012475-01
Euro OTC	Tetracaine	1512022	22299	45	20160128*
Euro OTC	Tetracaine	2304012	26661	40	20230508*
Fagron	Tetracaine	12L19-N10	20947	40	20130108
Fagron	Tetracaine	14A16-B04-292915	21650	60	20140205
Fagron	Tetracaine	14A16-B04-292916	21659	60	20140205
Fagron	Tetracaine	21L22-B01-216874	26081	40	20220315
Fagron	Tetracaine	21L22-B01-216874	26081SI	20	20220315

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 445 spectra of 10 reference samples from the substance/substance group *Tetracaine*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.
- 152 517 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 580 spectra of 16 reference samples from the substance/substance group *Tetracaine*.
- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Tetracaine	1606009	22717	40
Euro OTC	Tetracaine	1609010	22858	40
Euro OTC	Tetracaine	1701035	23149	40
Euro OTC	Tetracaine	1708024	23736	40
Euro OTC	Tetracaine	1803002	24066	40
Euro OTC	Tetracaine	1805019	24135	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Tetracaine	1811021	24427	40
Euro OTC	Tetracaine	1903004	24451	40
Euro OTC	Tetracaine	1909021	24961	40
Euro OTC	Tetracaine	2107010	25883	50
Euro OTC	Tetracaine	2203018	26046	40
Euro OTC	Tetracaine	2308016	27071	40
Euro OTC	Tetracaine	2401016	27161	40
Euro OTC	Tetracaine	2107010	25883SI	10
Euro OTC	Tetracaine	2203018	26046SI	20
Euro OTC	Tetracaine	2304012	26661SI[†]	20

- 201 504 spectra from a total of 4031 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 625 spectra from 230 *Apo-Ident* customers from 174 batches from the substance/substance group *Tetracaine*.
- Among them are spectra of independent samples from 160 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tetracaine	1811021-01	1
	Tetracaine	21L22-B01-216874	1
	Tetracaine	2203018-02	4
	Tetracaine	2302016-01	1
	Tetracaine	2304012-01	5
	Tetracaine	2304012-02	2
	Tetracaine	2401016-01	2
Caelo	Tetracaine	14A16-B04	1
Caelo	Tetracaine	14A16-B04-290207	1
Caelo	Tetracaine	14A16-B04-292916	1
Caelo	Tetracaine	1512022-01	1
Caelo	Tetracaine	1516B06312783	1
Caelo	Tetracaine	160004	1
Caelo	Tetracaine	1606009-01	1
Caelo	Tetracaine	16a13-b07-318736	1
Caelo	Tetracaine	16A13-B07-318736	5
Caelo	Tetracaine	16E23-B04	1
Caelo	Tetracaine	1701035-01	1
Caelo	Tetracaine	171111706	1
Caelo	Tetracaine	17111705	1
Caelo	Tetracaine	17111706	5
Caelo	Tetracaine	17111713	2
Caelo	Tetracaine	17111713P-190909-1	1
Caelo	Tetracaine	17111714	3
Caelo	Tetracaine	17K13-B02-344448	1

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tetracaine	17K13-B02-347172	2
Caelo	Tetracaine	1803002-01	1
Caelo	Tetracaine	1805019-01	2
Caelo	Tetracaine	1811021-01	2
Caelo	Tetracaine	18124097	1
Caelo	Tetracaine	18124905	1
Caelo	Tetracaine	19106602	5
Caelo	Tetracaine	19106605	1
Caelo	Tetracaine	192737004	3
Caelo	Tetracaine	192737006	1
Caelo	Tetracaine	192737008	1
Caelo	Tetracaine	20000160003	1
Caelo	Tetracaine	20000160009	2
Caelo	Tetracaine	20000160011	1
Caelo	Tetracaine	20003786004	14
Caelo	Tetracaine	20003786007	1
Caelo	Tetracaine	20003786012	8
Caelo	Tetracaine	2203018-01	2
Caelo	Tetracaine	T-290413-1	1
Caelo	Tetracaine	TC130621	1
Caeolo/Alliance	Tetracaine	20000160009	1
Caesar & Loretz GmbH...	Tetracaine	17111714	1
Caesar & Loretz GmbH...	Tetracaine	20000160003	1
Caesar & Loretz GmbH...	Tetracaine	17111706	1
Caesar & Loretz GmbH...	Tetracaine	20000160003	2
Caesar & Loretz GmbH	Tetracaine	18124906	1
Caesar & Loretz GmbH	Tetracaine	19106602	1
Caesar & Loretz GmbH	Tetracaine	192737004	1
Caesar & Loretz GmbH	Tetracaine	192737006	1
Caesar & Loretz GmbH	Tetracaine	20000160009	1
Caesar & Loretz GmbH	Tetracaine	20003786007	1
Caesar & Loretz/Noweda	Tetracaine	17111714	1
Ebert-Jacobi	Tetracaine	16J12-B06-327371	1
EuRho/ NOWEDA	Tetracaine	1811021-01	1
EuRho/ NOWEDA	Tetracaine	1903004-01	2
EuRho/ Phoenix	Tetracaine	1805019-01	1
EuRho/ Phoenix	Tetracaine	TC0090717	1
EuRho/AHD	Tetracaine	1811021-01	1
EuRho/GEHE	Tetracaine	1803002-01	1
EuRho/Jenne	Tetracaine	1909021-02	1
Eurho/noweda	Tetracaine	220301801	1
EuRho/Phoenix	Tetracaine	1909021-02	1
Eurho/Phönix	Tetracaine	1909021-01	1
EuRho	Tetracaine	220301801	1
EuRho	Tetracaine	519Q-04004	1
Euro OTC	Tetracaine	10887133	1
Euro OTC	Tetracaine	12081501	1
Euro OTC	Tetracaine	1312034-01	6
Euro OTC	Tetracaine	1405025-01	1
Euro OTC	Tetracaine	1405025-02	1
Euro OTC	Tetracaine	151022-01	1
Euro OTC	Tetracaine	1512022-01	4
Euro OTC	Tetracaine	160600-01	1
Euro OTC	Tetracaine	1606009-01	7
Euro OTC	Tetracaine	160901	1
Euro OTC	Tetracaine	1609010-01	15
Euro OTC	Tetracaine	1701035-01	10
Euro OTC	Tetracaine	170802401	3
Euro OTC	Tetracaine	1708024-01	14
Euro OTC	Tetracaine	1803002-01	16

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Tetracaine	18041809	1
Euro OTC	Tetracaine	180501901	2
Euro OTC	Tetracaine	1805019-01	10
Euro OTC	Tetracaine	1805019-02	2
Euro OTC	Tetracaine	181102101	8
Euro OTC	Tetracaine	1811021-01	29
Euro OTC	Tetracaine	19009021-02	1
Euro OTC	Tetracaine	1903001-02	1
Euro OTC	Tetracaine	1903004	2
Euro OTC	Tetracaine	190300401	1
Euro OTC	Tetracaine	1903004-01	22
Euro OTC	Tetracaine	1903004-02	3
Euro OTC	Tetracaine	1903004-03	2
Euro OTC	Tetracaine	1909021-01	33
Euro OTC	Tetracaine	1909021-02	1
Euro OTC	Tetracaine	1909021-21	2
Euro OTC	Tetracaine	19K04-F07	1
Euro OTC	Tetracaine	19K04-F07-368617	1
Euro OTC	Tetracaine	2107010-01	26
Euro OTC	Tetracaine	2107070-01	2
Euro OTC	Tetracaine	2203018-01	26
Euro OTC	Tetracaine	2203018-02	17
Euro OTC	Tetracaine	2203018-16	1
Euro OTC	Tetracaine	2304012-01	2
Euro OTC	Tetracaine	3081701	1
Euro OTC	Tetracaine	TC0010118	1
Euro OTC	Tetracaine	TC0041018	1
Euro OTC	Tetracaine	TC0091115	1
Euro/Noweda	Tetracaine	1805019-01	2
Euro/Phönix	Tetracaine	1903004-02	1
Fag	Tetracaine	16A13-B07-322947	1
Fagro/Noweda	Tetracaine	19A15-B01-361269	1
Fagron	Tetracaine		2
Fagron	Tetracaine	11D07-N20	1
Fagron	Tetracaine	11G12-N13	3
Fagron	Tetracaine	11l01-N09	1
Fagron	Tetracaine	11L09-N03	3
Fagron	Tetracaine	12F26-NO5	1
Fagron	Tetracaine	12f29-n05	1
Fagron	Tetracaine	12F29-N05	7
Fagron	Tetracaine	12H23-N07	1
Fagron	Tetracaine	12L19-N10	5
Fagron	Tetracaine	13D30-N11	2
Fagron	Tetracaine	14A16-B04	1
Fagron	Tetracaine	14A16-B04-2490207	1
Fagron	Tetracaine	14a16-b04-290208	1
Fagron	Tetracaine	14A16-B04-290208	3
Fagron	Tetracaine	14A16-B04-290209	1
Fagron	Tetracaine	14A16-B04-292916	1
Fagron	Tetracaine	14G30-B08	2
Fagron	Tetracaine	14g30-b08-297305	1
Fagron	Tetracaine	14G30-B08-297305	1
Fagron	Tetracaine	14g30-b08-297306	1
Fagron	Tetracaine	14G30-B08-297306	2
Fagron	Tetracaine	14G30-B08-297307	1
Fagron	Tetracaine	14K03-B02	1
Fagron	Tetracaine	14K03B02303178	1
Fagron	Tetracaine	14K03-B02-303178	1
Fagron	Tetracaine	14K03-B02-303179	2
Fagron	Tetracaine	15/16-B06-312783	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Tetracaine	15/16-B06-316260	1
Fagron	Tetracaine	1516-B06-316259	1
Fagron	Tetracaine	1516-B06-316260	1
Fagron	Tetracaine	15D01-B03-306258	1
Fagron	Tetracaine	15G30-B04-312060	1
Fagron	Tetracaine	16A13-B07-318736	5
Fagron	Tetracaine	16A13-B07-322947	2
Fagron	Tetracaine	16E23-B04-323269	1
Fagron	Tetracaine	16G29-B02-325569	4
Fagron	Tetracaine	16G29B02325570	2
Fagron	Tetracaine	16G29-B02-325570	1
Fagron	Tetracaine	16J12-B06	1
Fagron	Tetracaine	16J12-B06-327371	1
Fagron	Tetracaine	16J12-B06-329087	2
Fagron	Tetracaine	17184083	2
Fagron	Tetracaine	17E18-B02-337216	3
Fagron	Tetracaine	17E18-B02-337217	2
Fagron	Tetracaine	17K13-B02	1
Fagron	Tetracaine	17K13-B02-34172	1
Fagron	Tetracaine	17K13-B02-344448	7
Fagron	Tetracaine	17K13-B02-347172	7
Fagron	Tetracaine	18104050	1
Fagron	Tetracaine	18C26-B01-350472	1
Fagron	Tetracaine	19A15-B01	2
Fagron	Tetracaine	19A15-B010	2
Fagron	Tetracaine	19A15-B01-361263	2
Fagron	Tetracaine	19A15-B01-361269	5
Fagron	Tetracaine	19K04-F0-366996	1
Fagron	Tetracaine	19K04-F07	2
Fagron	Tetracaine	19K04-F07-0366996	1
Fagron	Tetracaine	19K04-F07-366996	4
Fagron	Tetracaine	19K04-F07-3669966	1
Fagron	Tetracaine	19K04-F07-368617	2
Fagron	Tetracaine	19K04-F07-369725	2
Fagron	Tetracaine	20E20-F06	3
Fagron	Tetracaine	20E20-F06-371444	3
Fagron	Tetracaine	20H28-U01-009031	1
Fagron	Tetracaine	20K16-F03-376067	1
Fagron	Tetracaine	21G10-B23-213654	1
Fagron	Tetracaine	21G10-B23-216782	4
Fagron	Tetracaine	21L22-B01-215564	4
Fagron	Tetracaine	21L22-B01-216874	1
Fagron	Tetracaine	2203018-02	3
Fagron	Tetracaine	2913Q-07165	1
Fagron	Tetracaine	3465093	1
Fagron	Tetracaine	5111202	1
Fagron	Tetracaine	9K04-F07-369725	1
Fagron	Tetracaine	F07-3697205	1
Fagron	Tetracaine	TC0041018	1
Fagron	Tetracaine	TC0070716	1
Fagron	Tetracaine	TC0090913	2
Fagron	Tetracaine	TC0140719	2
Fargon/AHD	Tetracaine	17K13-B02-347172	1
Fargon/Gehe	Tetracaine	18C26-B01-350472	1
Fargon/Gehe	Tetracaine	18c26-B01-355789	1
Faron	Tetracaine	15D01-B03-306258	2
Fragon/ Gehe	Tetracaine	18C26-B01-350472	1
Fragon/ Phönix	Tetracaine	19a15b01361263	1
GEHE 02.12.2014	Tetracaine	14A16-B04-290208	2
GEHE 04.05	Tetracaine	1405025-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
GEHE	Tetracaine	16G29-B02-325569	1
Gehe	Tetracaine	170103501	1
Gehe	Tetracaine	1805019-01	2
Gehe	Tetracaine	1811021-01	1
GEHE	Tetracaine	18C26-B01	1
Gehe	Tetracaine	21L22-B01-222760	1
gehe	Tetracaine	21L22-B01-222760	2
Gehe	Tetracaine	2304012-01	1
Geilenkirchen	Tetracaine	1805019-01	2
Hepart	Tetracaine	15G30-B04-310590	1
Jenne	Tetracaine	2203018-02	1
Noweda, EuRho	Tetracaine	2203018-01	1
Noweda/Fargon	Tetracaine	16/12-B06-329087	1
Noweda	Tetracaine	19A15-B01-361269	3
Phoenix 07.10.14	Tetracaine	14A16-B04-292916	1
Phoenix Goettin	Tetracaine	14G30-B08-297306	1
phoenix	Tetracaine	14A16B04290207	2
Phoenix	Tetracaine	1811021-01	1
Phoenix	Tetracaine	19k04-f07366996	1
Phoenix	Tetracaine	19k04-f07-366996	1
Phoenix	Tetracaine	19k04-f07369725	1
Phoenix	Tetracaine	20e20-f06-371444	1
Phoenix	Tetracaine	3118	1
Phönix Gotha	Tetracaine	10F11N04	1
Phönix	Tetracaine	11g12-n13	1
Phönix	Tetracaine	1303018-01	1
Phönix	Tetracaine	1312034-01	2
PHÖNIX	Tetracaine	20003786004	1
Phönix	Tetracaine	2304012-01	1
Phönix	Tetracaine	3465093	1
Rondell Apotheke	Tetracaine	1312034-01	1
Sanacorp	Tetracaine	1803002-01	1
Sanacorp	Tetracaine	1805019-01	1
sanacorp	Tetracaine	2203018-02	1
Sanacorp	Tetracaine	2304012-01	1
Sanacorp	Tetracaine	2308016-01	2
Sanacorp	Tetracaine	2401016-01	2
Sanacorp	Tetracaine	F07-3669906	1
Siegfried / Gehe	Tetracaine	18C26-B01-350472	1
siehe Lennartz	Tetracaine	sieheLennartz	1
tetracain	Tetracaine	1903004-03	1

- 235 442 spectra from 1515 *Apo-Ident* customers from a total of 49 087 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tetracaine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tetracaine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	445	0	152 517
Type B	0	580	0	201 504
Type C	0	625	0	235 442

The substance/substance group *Tetracaine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6517 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.9655 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 99.0400 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20947	21603	10.06	163.24
21603	21603	0.00	161.77
21650	22299	6.24	164.77
21659	21603	7.04	165.13
22299	22299	0.00	164.86
23321	23321	0.00	165.00
24255	24255	0.00	164.16
26081	24255	10.86	164.23
26661	26661	0.00	162.03

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tetracaine hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20037-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tetracaine hydrochloride; Tetracaini hydrochloridum

Special notes

When selecting the *Tetracaine hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tetracaine hydrochloride	8	20	386

Second-stage model

For differentiation of the substance/substance group *Tetracaine hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tetracaine hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	168.23	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tetracaine hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tetracaine hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Tetracaine hydrochloride	12019822	20924	40	20120228
Caelo	Tetracaine hydrochloride	15437108	23163	40	20160211
Euro OTC	Tetracaine hydrochloride	1506040	21845	60	20150713*
Euro OTC	Tetracaine hydrochloride	1512019	22285	45	20151228*
Euro OTC	Tetracaine hydrochloride	1612005	22912	40	20170112*
Euro OTC	Tetracaine hydrochloride	1807017	24141	40	20180730*
Fagron	Tetracaine hydrochloride	15K04-B03-322151	23162	40	20160112
Fagron	Tetracaine hydrochloride	16G28-B03-327368	23500	40	20160826

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 345 spectra of 8 reference samples from the substance/substance group *Tetracaine hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 617 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 910 spectra of 26 reference samples from the substance/substance group *Tetracaine hydrochloride*.

- Among them are spectra of independent samples from 20 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Tetracaine hydrochloride	190119	24561	40
Caelo	Tetracaine hydrochloride	22001496	26239	40
Euro OTC	Tetracaine hydrochloride	1607031	22708	40
Euro OTC	Tetracaine hydrochloride	1706018	23558	40
Euro OTC	Tetracaine hydrochloride	1712012	23886	40
Euro OTC	Tetracaine hydrochloride	1310006	23910	40
Euro OTC	Tetracaine hydrochloride	1803001	24079	40
Euro OTC	Tetracaine hydrochloride	1812006	24448	40
Euro OTC	Tetracaine hydrochloride	1902015	24452	40
Euro OTC	Tetracaine hydrochloride	1907007	24783	40
Euro OTC	Tetracaine hydrochloride	1909024	24974	40
Euro OTC	Tetracaine hydrochloride	2001011	25105	40
Euro OTC	Tetracaine hydrochloride	2003053	25267	40
Euro OTC	Tetracaine hydrochloride	2010019	25470	40
Euro OTC	Tetracaine hydrochloride	2110008	25885	50
Euro OTC	Tetracaine hydrochloride	2207015	26267	40
Euro OTC	Tetracaine hydrochloride	2307022	26879	30
Euro OTC	Tetracaine hydrochloride	2405009	27347	40
Fagron	Tetracaine hydrochloride	22J19-B01-221586	26551	40
Fagron	Tetracaine hydrochloride	24H26-B01-002406	27384	40
Caelo	Tetracaine hydrochloride	22001496	26239SI	20
Euro OTC	Tetracaine hydrochloride	2110008	25885SI	10
Euro OTC	Tetracaine hydrochloride	2207015	26267SI	20
Euro OTC	Tetracaine hydrochloride	2405009	27347SI	20
Fagron	Tetracaine hydrochloride	22J19-B01-221586	26551SI	20
Fagron	Tetracaine hydrochloride	24H26-B01-002406	27384SI	20

- 201 174 spectra from a total of 4025 batches from further 838 substances. These spectra were

recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 2088 spectra from 718 *Apo-Ident* customers from 395 batches from the substance/substance group *Tetracaine hydrochloride*.
- Among them are spectra of independent samples from 383 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tetracaine hydrochloride	1902015-01	1
	Tetracaine hydrochloride	1909024-01	1
	Tetracaine hydrochloride	2110008-01	3
	Tetracaine hydrochloride	21120-B04-225868	1
	Tetracaine hydrochloride	22001496004	1
	Tetracaine hydrochloride	22001496010	2
	Tetracaine hydrochloride	22001496014	1
	Tetracaine hydrochloride	22001496015	2
	Tetracaine hydrochloride	2201496015	1
	Tetracaine hydrochloride	2207015-01	7
	Tetracaine hydrochloride	2207015-02	1
	Tetracaine hydrochloride	2207015-03	3
	Tetracaine hydrochloride	221630	1
	Tetracaine hydrochloride	2307022-01	4
	Tetracaine hydrochloride	2405009-01	1
AHD/EuRho	Tetracaine hydrochloride	1902015-01	1
AHD	Tetracaine hydrochloride	15437121	1
AHD	Tetracaine hydrochloride	15A12-B03-308857	1
AHD	Tetracaine hydrochloride	18060602	1
AHD	Tetracaine hydrochloride	18060614	1
AHD	Tetracaine hydrochloride	2307022-01	1
AHD	Tetracaine hydrochloride	2405009-01	1
Alliance Health 05.0...	Tetracaine hydrochloride	13H21-B02-286559	1
Alliance Health 22.0...	Tetracaine hydrochloride	6093549	1
Alliance Health 30.0...	Tetracaine hydrochloride	1303012-01	2
Alliance Health	Tetracaine hydrochloride	14C18-B03-293967	1
Alliance Healthcare	Tetracaine hydrochloride	12H24-N05	1
Alliance	Tetracaine hydrochloride	220715-02	1
Anzag	Tetracaine hydrochloride	1411019-01	1
Anzag	Tetracaine hydrochloride	14710369	1
Anzag	Tetracaine hydrochloride	17256705	1
apo-ident	Tetracaine hydrochloride	1706018-01	1
Apolda/Gehe	Tetracaine hydrochloride	1909024	1
BASF Fine Chemicals ...	Tetracaine hydrochloride	13155714	1
BASF Pharma S.A.	Tetracaine hydrochloride	1310006-01	1
BASF Pharma S.A.	Tetracaine hydrochloride	1409026-02	1
BASF Pharma	Tetracaine hydrochloride	1411019-01	1
BASF	Tetracaine hydrochloride	13K25-B04-290277	1
BASF	Tetracaine hydrochloride	14C18-B03-293967	1
Bomastus / Alliance ...	Tetracaine hydrochloride	16G28-B03-327368	2
Bombastus	Tetracaine hydrochloride	13H21-B02-286558	1
Bombastus	Tetracaine hydrochloride	1712012-01	2
Caelo	Tetracaine hydrochloride	10118210	2
Caelo	Tetracaine hydrochloride	10118211	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tetracaine hydrochloride	10118225	4
Caelo	Tetracaine hydrochloride	1110010-01	1
Caelo	Tetracaine hydrochloride	1110010-02	2
Caelo	Tetracaine hydrochloride	1110010-07	1
Caelo	Tetracaine hydrochloride	12019802	5
Caelo	Tetracaine hydrochloride	12019810	5
Caelo	Tetracaine hydrochloride	12019812	3
Caelo	Tetracaine hydrochloride	12019815	1
Caelo	Tetracaine hydrochloride	12019816	11
Caelo	Tetracaine hydrochloride	12019820	1
Caelo	Tetracaine hydrochloride	12019822	6
Caelo	Tetracaine hydrochloride	1207001-01	1
Caelo	Tetracaine hydrochloride	1260917/15437119	1
Caelo	Tetracaine hydrochloride	12H24-N05	1
Caelo	Tetracaine hydrochloride	1303012-01	1
Caelo	Tetracaine hydrochloride	1310006-01	1
Caelo	Tetracaine hydrochloride	1310006-02	1
Caelo	Tetracaine hydrochloride	1313012-01	1
Caelo	Tetracaine hydrochloride	13155703	1
Caelo	Tetracaine hydrochloride	13155705	3
Caelo	Tetracaine hydrochloride	13155706	10
Caelo	Tetracaine hydrochloride	13155711	7
Caelo	Tetracaine hydrochloride	13155714	2
Caelo	Tetracaine hydrochloride	13155716	2
Caelo	Tetracaine hydrochloride	13155720	2
Caelo	Tetracaine hydrochloride	13155724	4
Caelo	Tetracaine hydrochloride	13155727	6
Caelo	Tetracaine hydrochloride	13K25-B04-290276	1
Caelo	Tetracaine hydrochloride	1405026-01	1
Caelo	Tetracaine hydrochloride	1409026-02	3
Caelo	Tetracaine hydrochloride	1411019-01	4
Caelo	Tetracaine hydrochloride	14c18-b03-293966	1
Caelo	Tetracaine hydrochloride	14C18-B03-300199	1
Caelo	Tetracaine hydrochloride	14C18-B03-300200	1
Caelo	Tetracaine hydrochloride	14G14-B08	1
Caelo	Tetracaine hydrochloride	14G14-B08-300198	1
Caelo	Tetracaine hydrochloride	15/16-B06-312783	1
Caelo	Tetracaine hydrochloride	150604001	1
Caelo	Tetracaine hydrochloride	1506040-01	2
Caelo	Tetracaine hydrochloride	150604002	1
Caelo	Tetracaine hydrochloride	15079501	2
Caelo	Tetracaine hydrochloride	15079507	1
Caelo	Tetracaine hydrochloride	1508040-01	1
Caelo	Tetracaine hydrochloride	1512019-01	3
Caelo	Tetracaine hydrochloride	1512019-02	1
Caelo	Tetracaine hydrochloride	15196102	5
Caelo	Tetracaine hydrochloride	15196103	6
Caelo	Tetracaine hydrochloride	15196104	2
Caelo	Tetracaine hydrochloride	15356902	2
Caelo	Tetracaine hydrochloride	1537109	1
Caelo	Tetracaine hydrochloride	15437102	1
Caelo	Tetracaine hydrochloride	15437104	14
Caelo	Tetracaine hydrochloride	15437106	3
Caelo	Tetracaine hydrochloride	15437107	2
Caelo	Tetracaine hydrochloride	15437108	4
Caelo	Tetracaine hydrochloride	15437109	12
Caelo	Tetracaine hydrochloride	15437114	12
Caelo	Tetracaine hydrochloride	15437117	6
Caelo	Tetracaine hydrochloride	15437118	2
Caelo	Tetracaine hydrochloride	15437119	18

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tetracaine hydrochloride	15437120	2
Caelo	Tetracaine hydrochloride	15437121	10
Caelo	Tetracaine hydrochloride	15437122	3
Caelo	Tetracaine hydrochloride	15H24-B03-311450	1
Caelo	Tetracaine hydrochloride	15K04-B03-318368	2
Caelo	Tetracaine hydrochloride	15K04-B03-318369	1
Caelo	Tetracaine hydrochloride	15K04-B03-328163	1
Caelo	Tetracaine hydrochloride	1607031-01	8
Caelo	Tetracaine hydrochloride	161200501	1
Caelo	Tetracaine hydrochloride	1612005-01	3
Caelo	Tetracaine hydrochloride	16G25-B03-332099	1
Caelo	Tetracaine hydrochloride	16G28-B03-332099	2
Caelo	Tetracaine hydrochloride	170601801	1
Caelo	Tetracaine hydrochloride	1706018-01	1
Caelo	Tetracaine hydrochloride	17114181	1
Caelo	Tetracaine hydrochloride	171201201	1
Caelo	Tetracaine hydrochloride	1712012-01	3
Caelo	Tetracaine hydrochloride	17256703	6
Caelo	Tetracaine hydrochloride	17256704	5
Caelo	Tetracaine hydrochloride	17256705	9
Caelo	Tetracaine hydrochloride	17G03-B07	1
Caelo	Tetracaine hydrochloride	17G03-B07-338538	2
Caelo	Tetracaine hydrochloride	17G03-B07-345008	2
Caelo	Tetracaine hydrochloride	17G03-B07-346693	1
Caelo	Tetracaine hydrochloride	1803001-01	16
Caelo	Tetracaine hydrochloride	1805019-01	1
Caelo	Tetracaine hydrochloride	18060602	20
Caelo	Tetracaine hydrochloride	18060603	6
Caelo	Tetracaine hydrochloride	18060604	4
Caelo	Tetracaine hydrochloride	18060606	1
Caelo	Tetracaine hydrochloride	18060609	2
Caelo	Tetracaine hydrochloride	18060610	1
Caelo	Tetracaine hydrochloride	18060612	10
Caelo	Tetracaine hydrochloride	18060613	1
Caelo	Tetracaine hydrochloride	18060614	5
Caelo	Tetracaine hydrochloride	18060619	2
Caelo	Tetracaine hydrochloride	18060620	8
Caelo	Tetracaine hydrochloride	18060621	3
Caelo	Tetracaine hydrochloride	18120006-01	1
Caelo	Tetracaine hydrochloride	1812006-01	3
Caelo	Tetracaine hydrochloride	18J03-B05	2
Caelo	Tetracaine hydrochloride	18J03-B05-361978	2
Caelo	Tetracaine hydrochloride	1901190002	1
Caelo	Tetracaine hydrochloride	190119001	9
Caelo	Tetracaine hydrochloride	190119002	3
Caelo	Tetracaine hydrochloride	190119003	1
Caelo	Tetracaine hydrochloride	19011901	7
Caelo	Tetracaine hydrochloride	19011903	8
Caelo	Tetracaine hydrochloride	19011903P-190909-2	1
Caelo	Tetracaine hydrochloride	19011906	3
Caelo	Tetracaine hydrochloride	19011907	9
Caelo	Tetracaine hydrochloride	19011908	9
Caelo	Tetracaine hydrochloride	20000156001	5
Caelo	Tetracaine hydrochloride	20000156002	1
Caelo	Tetracaine hydrochloride	20000156003	5
Caelo	Tetracaine hydrochloride	20000156005	7
Caelo	Tetracaine hydrochloride	20000156006	4
Caelo	Tetracaine hydrochloride	20000156008	7
Caelo	Tetracaine hydrochloride	200004176002	1
Caelo	Tetracaine hydrochloride	2000156003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tetracaine hydrochloride	2000156005	1
Caelo	Tetracaine hydrochloride	2000156008	1
Caelo	Tetracaine hydrochloride	20004176003	9
Caelo	Tetracaine hydrochloride	20004176004	8
Caelo	Tetracaine hydrochloride	20004176006	4
Caelo	Tetracaine hydrochloride	20004176007	1
Caelo	Tetracaine hydrochloride	20004176008	9
Caelo	Tetracaine hydrochloride	20004176011	2
Caelo	Tetracaine hydrochloride	20004176012	3
Caelo	Tetracaine hydrochloride	20004176013	3
Caelo	Tetracaine hydrochloride	20004176015	4
Caelo	Tetracaine hydrochloride	20004176016	2
Caelo	Tetracaine hydrochloride	20004176019	3
Caelo	Tetracaine hydrochloride	20004176020	3
Caelo	Tetracaine hydrochloride	20004176021	1
Caelo	Tetracaine hydrochloride	2003053-01	1
Caelo	Tetracaine hydrochloride	2110008-01	1
Caelo	Tetracaine hydrochloride	22001496003	1
Caelo	Tetracaine hydrochloride	22001496004	4
Caelo	Tetracaine hydrochloride	22001496005	2
Caelo	Tetracaine hydrochloride	2201496004	1
Caelo	Tetracaine hydrochloride	259/22	1
Caelo	Tetracaine hydrochloride	27111305	1
Caelo	Tetracaine hydrochloride	4176002	1
Caelo	Tetracaine hydrochloride	6093549	1
Caelo	Tetracaine hydrochloride	700216-0001	1
Caelo	Tetracaine hydrochloride	9070003	2
Caesar & Loretz GmbH...	Tetracaine hydrochloride	20004176003	1
Caesar & Loretz GmbH...	Tetracaine hydrochloride	22001496010	2
Caesar & Loretz GmbH/E	Tetracaine hydrochloride	20004176003	1
Caesar & Loretz GmbH...	Tetracaine hydrochloride	F10-3708006	1
Caesar & Loretz GmbH...	Tetracaine hydrochloride	TH0060219	1
Caesar & Loretz GmbH/Gehe	Tetracaine hydrochloride	190119001	1
Caesar & Loretz GmbH/Gehe	Tetracaine hydrochloride	1909024-02	2
Caesar & Loretz GmbH...	Tetracaine hydrochloride	19011908	2
Caesar & Loretz GmbH...	Tetracaine hydrochloride	18060614	1
Caesar & Loretz GmbH...	Tetracaine hydrochloride	18060621	1
Caesar & Loretz GmbH...	Tetracaine hydrochloride	20000156002	1
Caesar & Loretz GmbH...	Tetracaine hydrochloride	18060619	1
Caesar & Loretz GmbH...	Tetracaine hydrochloride	18060620	1
Caesar & Loretz GmbH...	Tetracaine hydrochloride	190119002	2
Caesar & Loretz GmbH	Tetracaine hydrochloride	17G03-B07-351509	1
Caesar & Loretz GmbH	Tetracaine hydrochloride	18060604	1
Caesar & Loretz GmbH	Tetracaine hydrochloride	18060610	1
Caesar & Loretz GmbH	Tetracaine hydrochloride	18060612	4
Caesar & Loretz GmbH	Tetracaine hydrochloride	18060619	1
Caesar & Loretz GmbH	Tetracaine hydrochloride	18060621	1
Caesar & Loretz GmbH	Tetracaine hydrochloride	190119001	2
Caesar & Loretz GmbH	Tetracaine hydrochloride	190119002	1
Caesar & Loretz GmbH	Tetracaine hydrochloride	190119003	2
Caesar & Loretz GmbH	Tetracaine hydrochloride	19011901	5
Caesar & Loretz GmbH	Tetracaine hydrochloride	19011902	1
Caesar & Loretz GmbH	Tetracaine hydrochloride	19011903	5
Caesar & Loretz GmbH	Tetracaine hydrochloride	19011906	1
Caesar & Loretz GmbH	Tetracaine hydrochloride	19011907	5
Caesar & Loretz GmbH	Tetracaine hydrochloride	19011908	5
Caesar & Loretz GmbH	Tetracaine hydrochloride	20000156001	1
Caesar & Loretz GmbH	Tetracaine hydrochloride	20000156002	1
Caesar & Loretz GmbH	Tetracaine hydrochloride	20000156005	1
Caesar & Loretz GmbH	Tetracaine hydrochloride	20000156006	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Tetracaine hydrochloride	20000156008	2
Caesar & Loretz GmbH	Tetracaine hydrochloride	20004176003	5
Caesar & Loretz GmbH	Tetracaine hydrochloride	20004176004	6
Caesar & Loretz GmbH	Tetracaine hydrochloride	20004176006	4
Caesar & Loretz GmbH	Tetracaine hydrochloride	20004176007	2
Caesar & Loretz GmbH	Tetracaine hydrochloride	20004176011	1
Caesar & Loretz GmbH	Tetracaine hydrochloride	20004176012	2
Caesar & Loretz GmbH	Tetracaine hydrochloride	20004176013	1
Caesar & Loretz GmbH	Tetracaine hydrochloride	20004176015	2
Caesar & Loretz GmbH	Tetracaine hydrochloride	20004176019	2
Caesar & Loretz GmbH	Tetracaine hydrochloride	20004176020	2
Caesar & Loretz GmbH	Tetracaine hydrochloride	22001496010	2
Caesar & Loretz GmbH	Tetracaine hydrochloride	TH0100718	1
Caesar & Loretz	Tetracaine hydrochloride	1803001-01	1
Caesar & Loretz	Tetracaine hydrochloride	18060609	1
Caesar Loretz	Tetracaine hydrochloride	190229001	1
Caesar Loretz	Tetracaine hydrochloride	20000156006	1
Calo/AHD	Tetracaine hydrochloride	13155727	1
Ebert-Jacobi	Tetracaine hydrochloride	15K04-B03-328163	1
Ebert-Jacobi	Tetracaine hydrochloride	1612005-01	1
EuRho / Fiebig	Tetracaine hydrochloride	2010019-01	1
EuRho Anzag	Tetracaine hydrochloride	1207001-01	1
EuRho/ NOWEDA	Tetracaine hydrochloride	14G14-B08-300198	1
EuRho/ Noweda	Tetracaine hydrochloride	1803001-01	3
EuRho/ Phönix	Tetracaine hydrochloride	1612002-01	1
EuRho/	Tetracaine hydrochloride	1712012-01	2
EuRho/AHD	Tetracaine hydrochloride	1909024-01	1
EuRho/AHD	Tetracaine hydrochloride	2010019-02	1
EuRho/Alliance	Tetracaine hydrochloride	2001011-01	1
EuRho/Gehe	Tetracaine hydrochloride	1909024-01	1
EuRho/Noweda	Tetracaine hydrochloride	1706018-01	1
EuRho/Phoenix	Tetracaine hydrochloride	2110008-01	2
Eurho/Phönix	Tetracaine hydrochloride	2003053-01	1
Eurho/Phönix	Tetracaine hydrochloride	2010019-01	1
Eurho/Phönix	Tetracaine hydrochloride	211000801	1
EuRho/Sanacorp	Tetracaine hydrochloride	1909024-02	1
EuRho/Sanacorp	Tetracaine hydrochloride	2001011-01	1
EuRho	Tetracaine hydrochloride	1106035-01	2
EuRho	Tetracaine hydrochloride	1110010-01	2
EuRho	Tetracaine hydrochloride	1110010-02	1
EuRho	Tetracaine hydrochloride	1615I-02039	1
EuRho	Tetracaine hydrochloride	1712012-01	2
euRho	Tetracaine hydrochloride	1803001-01	1
EuRho	Tetracaine hydrochloride	1803001-01	1
EuRho	Tetracaine hydrochloride	1902015-01	1
EuRho	Tetracaine hydrochloride	1909024-02	2
EuRho	Tetracaine hydrochloride	2001011-01	1
EuRho	Tetracaine hydrochloride	2003053-01	2
EuRho	Tetracaine hydrochloride	2010019-01	2
EuRho	Tetracaine hydrochloride	2906009V-04	1
EuRho	Tetracaine hydrochloride	TH0060219	1
Euro CT Phönix	Tetracaine hydrochloride	1207001-02	1
Euro ETC / Phönix	Tetracaine hydrochloride	2110008-01	1
Euro OT/Phönix	Tetracaine hydrochloride	TH0030315	1
Euro OTC	Tetracaine hydrochloride		1
Euro OTC	Tetracaine hydrochloride	1011-012	1
Euro OTC	Tetracaine hydrochloride	10416THCL	1
Euro OTC	Tetracaine hydrochloride	1106035	1
Euro OTC	Tetracaine hydrochloride	1106035-01	1
Euro OTC	Tetracaine hydrochloride	1110010-01	5

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Tetracaine hydrochloride	1110010-02	6
Euro OTC	Tetracaine hydrochloride	11110010-02	1
Euro OTC	Tetracaine hydrochloride	1207001-01	8
Euro OTC	Tetracaine hydrochloride	1207001-02	8
Euro OTC	Tetracaine hydrochloride	130301201	1
Euro OTC	Tetracaine hydrochloride	1303012-01	21
Euro OTC	Tetracaine hydrochloride	1310006-01	18
Euro OTC	Tetracaine hydrochloride	1310006-02	2
Euro OTC	Tetracaine hydrochloride	13155710	4
Euro OTC	Tetracaine hydrochloride	13509155	1
Euro OTC	Tetracaine hydrochloride	1404026-02	1
Euro OTC	Tetracaine hydrochloride	1405025-01	1
Euro OTC	Tetracaine hydrochloride	140502601	1
Euro OTC	Tetracaine hydrochloride	1405026-01	18
Euro OTC	Tetracaine hydrochloride	1405026-02	1
Euro OTC	Tetracaine hydrochloride	1405026-04	6
Euro OTC	Tetracaine hydrochloride	1409026	1
Euro OTC	Tetracaine hydrochloride	14090-26	1
Euro OTC	Tetracaine hydrochloride	140902601	1
Euro OTC	Tetracaine hydrochloride	1409026-01	12
Euro OTC	Tetracaine hydrochloride	140902602	1
Euro OTC	Tetracaine hydrochloride	1409026-02	12
Euro OTC	Tetracaine hydrochloride	1411019	1
Euro OTC	Tetracaine hydrochloride	141101901	1
Euro OTC	Tetracaine hydrochloride	1411019-01	26
Euro OTC	Tetracaine hydrochloride	14G14-B08-300202	1
Euro OTC	Tetracaine hydrochloride	150604001	1
Euro OTC	Tetracaine hydrochloride	1506040-01	29
Euro OTC	Tetracaine hydrochloride	1506040-02	7
Euro OTC	Tetracaine hydrochloride	15120019-01	1
Euro OTC	Tetracaine hydrochloride	1512019-01	32
Euro OTC	Tetracaine hydrochloride	151-2019-01	1
Euro OTC	Tetracaine hydrochloride	1512019-02	2
Euro OTC	Tetracaine hydrochloride	1603026-01	1
Euro OTC	Tetracaine hydrochloride	1607031	1
Euro OTC	Tetracaine hydrochloride	1607031_01	1
Euro OTC	Tetracaine hydrochloride	160703101	2
Euro OTC	Tetracaine hydrochloride	1607031-01	39
Euro OTC	Tetracaine hydrochloride	1607032-01	1
Euro OTC	Tetracaine hydrochloride	161200501	4
Euro OTC	Tetracaine hydrochloride	1612005-01	38
Euro OTC	Tetracaine hydrochloride	1612005-015445	1
Euro OTC	Tetracaine hydrochloride	170323181	1
Euro OTC	Tetracaine hydrochloride	1706018-01	22
Euro OTC	Tetracaine hydrochloride	17081503	1
Euro OTC	Tetracaine hydrochloride	17114181	1
Euro OTC	Tetracaine hydrochloride	171201201	1
Euro OTC	Tetracaine hydrochloride	1712012-01	26
Euro OTC	Tetracaine hydrochloride	171212-01	1
Euro OTC	Tetracaine hydrochloride	18003001-01	1
Euro OTC	Tetracaine hydrochloride	1803001	1
Euro OTC	Tetracaine hydrochloride	180300101	10
Euro OTC	Tetracaine hydrochloride	1803001-01	48
Euro OTC	Tetracaine hydrochloride	1803001-1	1
Euro OTC	Tetracaine hydrochloride	180701701	2
Euro OTC	Tetracaine hydrochloride	1807017-01	8
Euro OTC	Tetracaine hydrochloride	18120006-01	1
Euro OTC	Tetracaine hydrochloride	1812006	2
Euro OTC	Tetracaine hydrochloride	181200601	2
Euro OTC	Tetracaine hydrochloride	1812006-01	33

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Tetracaine hydrochloride	18701701	1
Euro OTC	Tetracaine hydrochloride	1902012-01	2
Euro OTC	Tetracaine hydrochloride	1902015	1
Euro OTC	Tetracaine hydrochloride	1902015-01	33
Euro OTC	Tetracaine hydrochloride	1907007	1
Euro OTC	Tetracaine hydrochloride	1907007-01	14
Euro OTC	Tetracaine hydrochloride	1909024_01	1
Euro OTC	Tetracaine hydrochloride	1909024-0	1
Euro OTC	Tetracaine hydrochloride	190902401	1
Euro OTC	Tetracaine hydrochloride	1909024-01	74
Euro OTC	Tetracaine hydrochloride	1909024-02	17
Euro OTC	Tetracaine hydrochloride	1909024-21	1
Euro OTC	Tetracaine hydrochloride	19909024-01	1
Euro OTC	Tetracaine hydrochloride	20010019-01	1
Euro OTC	Tetracaine hydrochloride	2001011-01	16
Euro OTC	Tetracaine hydrochloride	2003053	1
Euro OTC	Tetracaine hydrochloride	200305301	1
Euro OTC	Tetracaine hydrochloride	2003053-01	39
Euro OTC	Tetracaine hydrochloride	2003053-02	4
Euro OTC	Tetracaine hydrochloride	2003053-03	1
Euro OTC	Tetracaine hydrochloride	2010010-01	1
Euro OTC	Tetracaine hydrochloride	2010019-01	45
Euro OTC	Tetracaine hydrochloride	2010019-02	14
Euro OTC	Tetracaine hydrochloride	2010091-01	1
Euro OTC	Tetracaine hydrochloride	201019-02	1
Euro OTC	Tetracaine hydrochloride	20160812-2	1
Euro OTC	Tetracaine hydrochloride	21071807	1
Euro OTC	Tetracaine hydrochloride	2110008-01	24
Euro OTC	Tetracaine hydrochloride	211008-01	1
Euro OTC	Tetracaine hydrochloride	2207015-01	5
Euro OTC	Tetracaine hydrochloride	2207015-02	1
Euro OTC	Tetracaine hydrochloride	24102014A	1
Euro OTC	Tetracaine hydrochloride	2906009V-03	1
Euro OTC	Tetracaine hydrochloride	3071716	1
Euro OTC	Tetracaine hydrochloride	3113M-02039	1
Euro OTC	Tetracaine hydrochloride	4811A-02039	1
Euro OTC	Tetracaine hydrochloride	5016Y-02039	1
Euro OTC	Tetracaine hydrochloride	6093547	1
Euro OTC	Tetracaine hydrochloride	Euro-OTC	1
Euro OTC	Tetracaine hydrochloride	TH0030315	1
Euro OTC	Tetracaine hydrochloride	TH00602019	1
Euro OTC	Tetracaine hydrochloride	TH0070816	1
Euro OTC	Tetracaine hydrochloride	TH0100718	2
Euro OTC	Tetracaine hydrochloride	TH0121219	2
Euro OTG Pharma	Tetracaine hydrochloride	1409026-02	1
Euro OTG/ AHD	Tetracaine hydrochloride	1706018-01	2
Euro OTG	Tetracaine hydrochloride	1207001-01	1
Euro/Phönix	Tetracaine hydrochloride	1506040-01	1
Euro	Tetracaine hydrochloride	1506040-01	1
euroct/gehe	Tetracaine hydrochloride	1405026-01	1
EuroTOC / Noweda	Tetracaine hydrochloride	131000601	2
EurRho/Noweda	Tetracaine hydrochloride	1712012-01	2
fag	Tetracaine hydrochloride	20G10-F07-373354	1
Fagreo / Sanacorp	Tetracaine hydrochloride	20A17F10370805	1
Fagro/Gehe	Tetracaine hydrochloride	16G28-B03-327368	2
Fagron	Tetracaine hydrochloride		1
Fagron	Tetracaine hydrochloride	10330837	1
Fagron	Tetracaine hydrochloride	10990834	3
Fagron	Tetracaine hydrochloride	10990837	3
Fagron	Tetracaine hydrochloride	10990841	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Tetracaine hydrochloride	10A29-N12	2
Fagron	Tetracaine hydrochloride	11/15-N12	1
Fagron	Tetracaine hydrochloride	11A31-N15	1
Fagron	Tetracaine hydrochloride	11C22-N04	1
Fagron	Tetracaine hydrochloride	12C22-N04	5
Fagron	Tetracaine hydrochloride	12H24-N05	12
Fagron	Tetracaine hydrochloride	12H24-N050696/1050	1
Fagron	Tetracaine hydrochloride	12H-N05	1
Fagron	Tetracaine hydrochloride	12K01-N04	7
Fagron	Tetracaine hydrochloride	1303012-01	1
Fagron	Tetracaine hydrochloride	13155711	1
Fagron	Tetracaine hydrochloride	13509149	2
Fagron	Tetracaine hydrochloride	13509155	1
Fagron	Tetracaine hydrochloride	13D11-N01	1
Fagron	Tetracaine hydrochloride	13D11-N07	12
Fagron	Tetracaine hydrochloride	13G02-N01	1
Fagron	Tetracaine hydrochloride	13H21-B02	2
Fagron	Tetracaine hydrochloride	13H21-B02-286558	3
Fagron	Tetracaine hydrochloride	13H21-B02-286559	1
Fagron	Tetracaine hydrochloride	13K25-B04	1
Fagron	Tetracaine hydrochloride	13k25-b04-290276	1
Fagron	Tetracaine hydrochloride	13K25-B04290276	1
Fagron	Tetracaine hydrochloride	13K25-B04-290276	3
Fagron	Tetracaine hydrochloride	13K25B04290277	1
Fagron	Tetracaine hydrochloride	13K25-B04-290278	1
Fagron	Tetracaine hydrochloride	13K25-Bo4-290276	1
Fagron	Tetracaine hydrochloride	1411019-01	2
Fagron	Tetracaine hydrochloride	1418-03-300199	1
Fagron	Tetracaine hydrochloride	14710369	1
Fagron	Tetracaine hydrochloride	14C18-B03	1
Fagron	Tetracaine hydrochloride	14C18-B03-293966	7
Fagron	Tetracaine hydrochloride	14C18-B03-293967	1
Fagron	Tetracaine hydrochloride	14C18-B03-300199	6
Fagron	Tetracaine hydrochloride	14C18-B03-300200	4
Fagron	Tetracaine hydrochloride	14C18-Bo3-300200	1
Fagron	Tetracaine hydrochloride	14c18d03300199	1
Fagron	Tetracaine hydrochloride	14G14B08300198	1
Fagron	Tetracaine hydrochloride	14G14-B08-300198	8
Fagron	Tetracaine hydrochloride	1506040-02	1
Fagron	Tetracaine hydrochloride	15A12B03308857	1
Fagron	Tetracaine hydrochloride	15A12-B03-308857	8
Fagron	Tetracaine hydrochloride	15H24-B03	3
Fagron	Tetracaine hydrochloride	15H24-B03-311450	6
Fagron	Tetracaine hydrochloride	15h24-b03-313594	1
Fagron	Tetracaine hydrochloride	15H24-B03-313594	6
Fagron	Tetracaine hydrochloride	15H24-B03-314243	1
Fagron	Tetracaine hydrochloride	15K04-B03	2
Fagron	Tetracaine hydrochloride	15K04-B03_322151	1
Fagron	Tetracaine hydrochloride	15K04-B03-318368	3
Fagron	Tetracaine hydrochloride	15K04B03318369	1
Fagron	Tetracaine hydrochloride	15K04-B03-318369	3
Fagron	Tetracaine hydrochloride	15K04-B03-321567	1
Fagron	Tetracaine hydrochloride	15K04-B03-321568	1
Fagron	Tetracaine hydrochloride	15K04-B03-322151	14
Fagron	Tetracaine hydrochloride	15K04-B03-328163	1
Fagron	Tetracaine hydrochloride	15K04-bo3-312151	1
Fagron	Tetracaine hydrochloride	1607031-01	1
Fagron	Tetracaine hydrochloride	16G28-B03	1
Fagron	Tetracaine hydrochloride	16G28-B03-327368	14
Fagron	Tetracaine hydrochloride	16G28-B03-327369	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Tetracaine hydrochloride	16G28-B03-328913	1
Fagron	Tetracaine hydrochloride	16G28-B03-330362	5
Fagron	Tetracaine hydrochloride	16G28-B03-330363	1
Fagron	Tetracaine hydrochloride	16G28-B03-332099	3
Fagron	Tetracaine hydrochloride	16G28-B03-334124	2
Fagron	Tetracaine hydrochloride	16G2-B03-327368	1
Fagron	Tetracaine hydrochloride	16G8-B03-327368	1
Fagron	Tetracaine hydrochloride	17114181	12
Fagron	Tetracaine hydrochloride	17G03_B07-351508	1
Fagron	Tetracaine hydrochloride	17G03-B07	8
Fagron	Tetracaine hydrochloride	17G03-B07-338538	7
Fagron	Tetracaine hydrochloride	17G03-B07-338539	4
Fagron	Tetracaine hydrochloride	17G03-B07-338540	1
Fagron	Tetracaine hydrochloride	17G03-B07-341319	1
Fagron	Tetracaine hydrochloride	17G03-B07-341853	4
Fagron	Tetracaine hydrochloride	17G03-B07-345008	7
Fagron	Tetracaine hydrochloride	17G03-B07-345009	3
Fagron	Tetracaine hydrochloride	17G03-B07-349367	5
Fagron	Tetracaine hydrochloride	17G03-B07-349368	2
Fagron	Tetracaine hydrochloride	17G03-B07-3515009	1
Fagron	Tetracaine hydrochloride	17G03-B07-351508	2
Fagron	Tetracaine hydrochloride	17G03-B07-351509	2
Fagron	Tetracaine hydrochloride	17G05-B04-341204	1
Fagron	Tetracaine hydrochloride	17Go3-B07-341853	1
Fagron	Tetracaine hydrochloride	1803001-01	1
Fagron	Tetracaine hydrochloride	1812006-01	1
Fagron	Tetracaine hydrochloride	18J03-B05	5
Fagron	Tetracaine hydrochloride	18J03-B05-356329	5
Fagron	Tetracaine hydrochloride	18J03-B05-356330	2
Fagron	Tetracaine hydrochloride	18J03-B05-358079	1
Fagron	Tetracaine hydrochloride	18J03B05358080	1
Fagron	Tetracaine hydrochloride	18J03-B05-358080	6
Fagron	Tetracaine hydrochloride	18J03-B05-359813	5
Fagron	Tetracaine hydrochloride	18J03-B05-359814	2
Fagron	Tetracaine hydrochloride	18J03-B05-359815	2
Fagron	Tetracaine hydrochloride	18J03-B05-361978	4
Fagron	Tetracaine hydrochloride	18J03-B05-361979	5
Fagron	Tetracaine hydrochloride	18J03-B05-362469	8
Fagron	Tetracaine hydrochloride	18J03-B05-362470	2
Fagron	Tetracaine hydrochloride	18J03-B05-362471	4
Fagron	Tetracaine hydrochloride	18J03-B05-58079	1
Fagron	Tetracaine hydrochloride	18j0-b05-358079	1
Fagron	Tetracaine hydrochloride	192021003	1
Fagron	Tetracaine hydrochloride	20A17-F10	3
Fagron	Tetracaine hydrochloride	20A17-F1008581264	1
Fagron	Tetracaine hydrochloride	20A17-F10-3708007	1
Fagron	Tetracaine hydrochloride	20A17-F10-370805	3
Fagron	Tetracaine hydrochloride	20A17-F10-370806	2
Fagron	Tetracaine hydrochloride	20A17-F10-370807	3
Fagron	Tetracaine hydrochloride	20G10-07-373352	1
Fagron	Tetracaine hydrochloride	20G10-F07	3
Fagron	Tetracaine hydrochloride	20G10-F07-372358	1
Fagron	Tetracaine hydrochloride	20G10-F07-373352	5
Fagron	Tetracaine hydrochloride	20G10F07373353	1
Fagron	Tetracaine hydrochloride	20G10-F07-373353	6
Fagron	Tetracaine hydrochloride	20G10-F07-373354	1
Fagron	Tetracaine hydrochloride	20G10-F07-374915	1
Fagron	Tetracaine hydrochloride	20G10-F07-374916	1
Fagron	Tetracaine hydrochloride	20L03-F02-377430	2
Fagron	Tetracaine hydrochloride	21120-B04-213603	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Tetracaine hydrochloride	212131/221630-0002	1
Fagron	Tetracaine hydrochloride	218I-02039	1
Fagron	Tetracaine hydrochloride	21I20-B04-213603	2
Fagron	Tetracaine hydrochloride	21I20-B04-213604	4
Fagron	Tetracaine hydrochloride	21120-B04-213604	1
Fagron	Tetracaine hydrochloride	221I20-B04-213603	1
Fagron	Tetracaine hydrochloride	2OA17-F10-370807	2
Fagron	Tetracaine hydrochloride	3413U02039	1
Fagron	Tetracaine hydrochloride	3913I-02039	1
Fagron	Tetracaine hydrochloride	4118A-02039	1
Fagron	Tetracaine hydrochloride	4313E-02039	1
Fagron	Tetracaine hydrochloride	6093547	2
Fagron	Tetracaine hydrochloride	6093549	1
Fagron	Tetracaine hydrochloride	715Q-02039	1
Fagron	Tetracaine hydrochloride	B05-3619708	2
Fagron	Tetracaine hydrochloride	F07-3733502	1
Fagron	Tetracaine hydrochloride	F10-3708005	1
Fagron	Tetracaine hydrochloride	F10-3708006	1
Fagron	Tetracaine hydrochloride	F10-3708007	1
Fagron	Tetracaine hydrochloride	TH0050520	2
Fagron	Tetracaine hydrochloride	TH0060721	1
Fagron	Tetracaine hydrochloride	TH0100718	6
Fargon / GEIBO	Tetracaine hydrochloride	21120-B04-213604	1
Fargon Services NL	Tetracaine hydrochloride	15K04-B03-322151	5
Fargon/AllianceH.	Tetracaine hydrochloride	17G03-B07-338538	1
Fargon/Noweda	Tetracaine hydrochloride	17G03-B07-345008	1
Fargron/ Sanacorp	Tetracaine hydrochloride	14C18-B03-300200	1
Fiebig/Calo	Tetracaine hydrochloride	17256704	1
Finze	Tetracaine hydrochloride	2906009-02	1
Gatt-Koller / Phoenix	Tetracaine hydrochloride	80/02140614	2
Gatt-Koller	Tetracaine hydrochloride	1803034	2
Gatt-Koller	Tetracaine hydrochloride	1900461	6
Gatt-Koller	Tetracaine hydrochloride	KNC1825J18	1
Gehe 07.07.2014	Tetracaine hydrochloride	13155706	1
Gehe amax	Tetracaine hydrochloride	1812006-01	1
gehe europharm	Tetracaine hydrochloride	201001901	1
Gehe	Tetracaine hydrochloride	1310006-01	1
Gehe	Tetracaine hydrochloride	13155711	2
Gehe	Tetracaine hydrochloride	15437119	1
Gehe	Tetracaine hydrochloride	15A12-B03-308857	1
Gehe	Tetracaine hydrochloride	15K04-B03-322151	1
GEHE	Tetracaine hydrochloride	1612005-01	1
GEHE	Tetracaine hydrochloride	1706018-01	1
GEHE	Tetracaine hydrochloride	17G03-B07-338540	1
Gehe	Tetracaine hydrochloride	1803001-01	1
GEHE	Tetracaine hydrochloride	18060602	2
GEHE	Tetracaine hydrochloride	18060614	2
Gehe	Tetracaine hydrochloride	1812006-01	1
Gehe	Tetracaine hydrochloride	1902015-01	1
Gehe	Tetracaine hydrochloride	1907007-01	1
Gehe	Tetracaine hydrochloride	1909024-01	1
Gehe	Tetracaine hydrochloride	200041	1
Gehe	Tetracaine hydrochloride	20004176008	1
Gehe	Tetracaine hydrochloride	2010019-02	1
Gehe	Tetracaine hydrochloride	2207015-02	1
Geibo/ Fargron	Tetracaine hydrochloride	15H24-B03-313594	1
Geibo/ Fargron	Tetracaine hydrochloride	17G03-B07-338538	1
Geibo	Tetracaine hydrochloride	2003053-01	1
Geibo	Tetracaine hydrochloride	22001496003	1
Geilenkirchen	Tetracaine hydrochloride	1812006-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Geilenkirchen	Tetracaine hydrochloride	1902015-01	2
Geilenkirchen	Tetracaine hydrochloride	1909024-01	1
Gutenberg-Apotheke	Tetracaine hydrochloride	13D11-N07	1
Hänseler	Tetracaine hydrochloride		4
Hänseler	Tetracaine hydrochloride	2018060021	1
Jenne	Tetracaine hydrochloride	13D11-No7	1
Kehr	Tetracaine hydrochloride	22001496010	1
Lamotte/3	Tetracaine hydrochloride	13155720	1
Noveda	Tetracaine hydrochloride	12H24-N05	1
Noweda 06.02.19 EK:7,84	Tetracaine hydrochloride	1807017-01	1
Noweda Taucha	Tetracaine hydrochloride	2110008-01	1
Noweda/ BASF Pharma ...	Tetracaine hydrochloride	12H24-N05	1
Noweda	Tetracaine hydrochloride	1106035-01	2
Noweda	Tetracaine hydrochloride	120700-02	1
Noweda	Tetracaine hydrochloride	1310006-01	1
Noweda	Tetracaine hydrochloride	1405026-04	2
Noweda	Tetracaine hydrochloride	14G14-B08	1
Noweda	Tetracaine hydrochloride	17G03-B07-351508	2
Noweda	Tetracaine hydrochloride	1812006-01	1
Noweda	Tetracaine hydrochloride	18J03-B05-359814	1
Noweda	Tetracaine hydrochloride	19011908	1
Noweda	Tetracaine hydrochloride	1909024-1	1
Noweda	Tetracaine hydrochloride	20004176012	1
Noweda	Tetracaine hydrochloride	211008-01	2
Noweda	Tetracaine hydrochloride	22001496004	1
Noweda	Tetracaine hydrochloride	2207015-01	1
Noweda	Tetracaine hydrochloride	2207015-02	1
Noweda	Tetracaine hydrochloride	22J19-B01-221586	1
Noweda	Tetracaine hydrochloride	TH0050520	1
Nutra / Noweda	Tetracaine hydrochloride	1803001-01	1
Orgamol Pharma	Tetracaine hydrochloride	6093547	1
Pala	Tetracaine hydrochloride	18J03-B05-356329	1
Phoenix 04.11.16 Pho...	Tetracaine hydrochloride	1607031-01	1
Phoenix 27.07.2019 6,98EUR	Tetracaine hydrochloride	1712012-01	1
Phoenix am 30.04.2014	Tetracaine hydrochloride	1310006-01	1
Phoenix Goettin	Tetracaine hydrochloride	1409026-01	1
Phoenix	Tetracaine hydrochloride	15437104	2
Phoenix	Tetracaine hydrochloride	1803001-01	1
Phoenix	Tetracaine hydrochloride	20004176004	1
Phoenix	Tetracaine hydrochloride	2003053-01	2
Phoenix	Tetracaine hydrochloride	2010019-01	1
Phoenix	Tetracaine hydrochloride	2110008-01	1
Phoenix	Tetracaine hydrochloride	2207015-01	1
Phoenix	Tetracaine hydrochloride	3058	1
Phönix /euro	Tetracaine hydrochloride	2003053-01	1
Phönix	Tetracaine hydrochloride	130301201	1
Phönix	Tetracaine hydrochloride	1310006-01	1
Phönix	Tetracaine hydrochloride	1405026-01	1
PHÖNIX	Tetracaine hydrochloride	15437109	1
phönix	Tetracaine hydrochloride	15437121	1
Phönix	Tetracaine hydrochloride	1612005-01	1
Phönix	Tetracaine hydrochloride	171201201	1
Phönix	Tetracaine hydrochloride	1812006-01	1
Phönix	Tetracaine hydrochloride	1902015-01	1
Phönix	Tetracaine hydrochloride	1909024-01	1
PHÖNIX	Tetracaine hydrochloride	2003053-02	1
Phönix	Tetracaine hydrochloride	2010019-01	1
PHönix	Tetracaine hydrochloride	2010019-01	1
Phönix	Tetracaine hydrochloride	2015E-02039	1
Phönix	Tetracaine hydrochloride	2207015-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Tetracaine hydrochloride	2207015-03	1
Phönix	Tetracaine hydrochloride	22J19-B01-221586	1
Phönix	Tetracaine hydrochloride	2405009-01	3
Sana 20.12.17 7.99	Tetracaine hydrochloride	1612005-01	2
Sanacorp, 21.02.17, …	Tetracaine hydrochloride	1607031-01	1
Sanacorp/EuRho	Tetracaine hydrochloride	18060604	1
Sanacorp	Tetracaine hydrochloride	1207001-02	1
Sanacorp	Tetracaine hydrochloride	1303012-01	1
Sanacorp	Tetracaine hydrochloride	1409026-01	1
Sanacorp	Tetracaine hydrochloride	15/AKD1	1
Sanacorp	Tetracaine hydrochloride	17G03-B07-341318	1
Sanacorp	Tetracaine hydrochloride	17G03-B07-341853	1
Sanacorp	Tetracaine hydrochloride	1803001-01	2
Sanacorp	Tetracaine hydrochloride	19011903	2
Sanacorp	Tetracaine hydrochloride	1902015-01	1
Sanacorp	Tetracaine hydrochloride	2001011-01	1
Sanacorp	Tetracaine hydrochloride	20A17-F10	2
Sanacorp	Tetracaine hydrochloride	20A17-F10-370806	1
Sanacorp	Tetracaine hydrochloride	20G10-F07-373352	2
Sanacorp	Tetracaine hydrochloride	2110008-01	1
Sanacorp	Tetracaine hydrochloride	21I20-B04-213603	1
Sanacorp	Tetracaine hydrochloride	22001496004	1
sanacorp	Tetracaine hydrochloride	2207015-02	1
Sanacorp	Tetracaine hydrochloride	2207015-03	1
Sanacorp	Tetracaine hydrochloride	F07-3733502	1
Sino Phyto	Tetracaine hydrochloride	12019816	1
Synopharm/Anzag	Tetracaine hydrochloride	2712Q-02039	1
VDl 26.09.14 12,00 euro	Tetracaine hydrochloride	1405026-01	1
Venkata NA / Gehe	Tetracaine hydrochloride	190119002	2
Venkata Narayana / Gehe	Tetracaine hydrochloride	1907007-01	1
Venkata/Noweda	Tetracaine hydrochloride	TH00602019	1
Venkata/Noweda	Tetracaine hydrochloride	TH0060219	1
Venkata/phoenix	Tetracaine hydrochloride	TH0100718	1

- 233 979 spectra from 1515 *Apo-Ident* customers from a total of 48 878 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tetracaine hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tetracaine hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	345	0	152 617
Type B	0	910	0	201 174
Type C	0	2059	29	233 979

The substance/substance group *Tetracaine hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.2609 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.3407 %)
Type C	100.0000 % (> 99.9007 %)	98.6111 % (> 98.4674 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20924	21845	7.27	209.21
21845	21845	0.00	207.88
22285	22285	0.00	207.88
22912	22912	0.00	207.59
23162	21845	7.59	207.94
23163	21845	8.85	207.37
23500	21845	7.02	206.77
24141	24141	0.00	203.97

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tetracycline hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20044-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tetracycline hydrochloride; Tetracyclini hydrochloridum

Special notes

When selecting the *Tetracycline hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tetracycline hydrochloride	8	7	185

Second-stage model

For differentiation of the substance/substance group *Tetracycline hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tetracycline hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Chlortetracycline hydrochloride	54.75	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tetracycline hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tetracycline hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Tetracycline hydrochloride	13201303	21427	60	20130807
Caelo	Tetracycline hydrochloride	13201303	21428	60	20130807
Caelo	Tetracycline hydrochloride	161167	22468	60	20160504*
Caelo	Tetracycline hydrochloride	15230712	22833	40	20150819
Caelo	Tetracycline hydrochloride	20003996010	26301	30	20201127
Caelo	Tetracycline hydrochloride	20003996010	26301SI	20	20201127
Euro OTC	Tetracycline hydrochloride	1302012-01	21079	40	1411585
Euro OTC	Tetracycline hydrochloride	1506012	21835	60	20150707*
Euro OTC	Tetracycline hydrochloride	2004023	25279	40	20200721*
Euro OTC	Tetracycline hydrochloride	2103015	25686	50	20210525*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 460 spectra of 10 reference samples from the substance/substance group *Tetracycline hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 502 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 320 spectra of 9 reference samples from the substance/substance group *Tetracycline hydrochloride*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Tetracycline hydrochloride	172858	23847	40
Caelo	Tetracycline hydrochloride	181986	24256	40
Caelo	Tetracycline hydrochloride	183083	24394	40
Euro OTC	Tetracycline hydrochloride	1603026	22545	40
Euro OTC	Tetracycline hydrochloride	1706020	23691	30
Euro OTC	Tetracycline hydrochloride	1811031	24450	40
Euro OTC	Tetracycline hydrochloride	2203017	26099	40
Euro OTC	Tetracycline hydrochloride	2103015	25686SI†	10
Euro OTC	Tetracycline hydrochloride	2203017	26099SI	40

- 201 764 spectra from a total of 4037 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1032 spectra from 504 *Apo-Ident* customers from 190 batches from the substance/substance group *Tetracycline hydrochloride*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 184 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tetracycline hydrochloride	21003348003	1
	Tetracycline hydrochloride	21003348008	1
	Tetracycline hydrochloride	21003348011	2
	Tetracycline hydrochloride	21003348015	1
	Tetracycline hydrochloride	21003348017	2
	Tetracycline hydrochloride	2103015-02	4
	Tetracycline hydrochloride	2203017-01	3
	Tetracycline hydrochloride	23000427002	1
	Tetracycline hydrochloride	23000427003	1
	Tetracycline hydrochloride	23000427005	6
	Tetracycline hydrochloride	23000427009	1
	Tetracycline hydrochloride	24000509004	1
	Tetracycline hydrochloride	24000509005	1
AHD	Tetracycline hydrochloride	21003348003	1
AHD	Tetracycline hydrochloride	23000427005	1
Aliance am 10.03.2014	Tetracycline hydrochloride	1302012-02	1
Alliance Health 22.0...	Tetracycline hydrochloride	13201307	1
Alliance Healthcare	Tetracycline hydrochloride	192021008	1
Anzag/euRho	Tetracycline hydrochloride		1
Bombastus	Tetracycline hydrochloride	1204039-02	1
Bombastus	Tetracycline hydrochloride	1603026-01	2
Bombastus	Tetracycline hydrochloride	1811031-01	1
Caeli / Phönix	Tetracycline hydrochloride	21003348002	1
Caelo	Tetracycline hydrochloride	1017A-02378	1
Caelo	Tetracycline hydrochloride	103201301	1
Caelo	Tetracycline hydrochloride	111002901	1
Caelo	Tetracycline hydrochloride	1160117	1
Caelo	Tetracycline hydrochloride	1204039	2
Caelo	Tetracycline hydrochloride	12138104	1
Caelo	Tetracycline hydrochloride	12138106	2
Caelo	Tetracycline hydrochloride	12353602	1
Caelo	Tetracycline hydrochloride	12353603	6
Caelo	Tetracycline hydrochloride	12353609	1
Caelo	Tetracycline hydrochloride	12353612	1
Caelo	Tetracycline hydrochloride	12353613	1
Caelo	Tetracycline hydrochloride	1302012-01	1
Caelo	Tetracycline hydrochloride	13201301	3
Caelo	Tetracycline hydrochloride	13201302	1
Caelo	Tetracycline hydrochloride	13201307	1
Caelo	Tetracycline hydrochloride	13201309	2
Caelo	Tetracycline hydrochloride	13F17-N03	1
Caelo	Tetracycline hydrochloride	13L10B02296956	1
Caelo	Tetracycline hydrochloride	1402030-01	1
Caelo	Tetracycline hydrochloride	14080605	2
Caelo	Tetracycline hydrochloride	14080606	4
Caelo	Tetracycline hydrochloride	1412007-01	2
Caelo	Tetracycline hydrochloride	1412007-03	3
Caelo	Tetracycline hydrochloride	14364601	1
Caelo	Tetracycline hydrochloride	14364604	3
Caelo	Tetracycline hydrochloride	14364612	3
Caelo	Tetracycline hydrochloride	14364614	1
Caelo	Tetracycline hydrochloride	14364616	2
Caelo	Tetracycline hydrochloride	14H06-B05-313591	1
Caelo	Tetracycline hydrochloride	1506012-01	4
Caelo	Tetracycline hydrochloride	151018-61	1
Caelo	Tetracycline hydrochloride	15230703	4
Caelo	Tetracycline hydrochloride	15230707	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tetracycline hydrochloride	15230711	1
Caelo	Tetracycline hydrochloride	15230714	1
Caelo	Tetracycline hydrochloride	15230715	5
Caelo	Tetracycline hydrochloride	15230717	3
Caelo	Tetracycline hydrochloride	15230720	3
Caelo	Tetracycline hydrochloride	1603026-01	3
Caelo	Tetracycline hydrochloride	1611617	1
Caelo	Tetracycline hydrochloride	16116701	3
Caelo	Tetracycline hydrochloride	16116704	1
Caelo	Tetracycline hydrochloride	16116706	6
Caelo	Tetracycline hydrochloride	16116708	1
Caelo	Tetracycline hydrochloride	16116709	5
Caelo	Tetracycline hydrochloride	16116714	2
Caelo	Tetracycline hydrochloride	16116715	8
Caelo	Tetracycline hydrochloride	16116720	2
Caelo	Tetracycline hydrochloride	16116721	9
Caelo	Tetracycline hydrochloride	166116709	1
Caelo	Tetracycline hydrochloride	170602001	3
Caelo	Tetracycline hydrochloride	1706020-01	6
Caelo	Tetracycline hydrochloride	172855809	1
Caelo	Tetracycline hydrochloride	17285801	12
Caelo	Tetracycline hydrochloride	17285802	1
Caelo	Tetracycline hydrochloride	17285803	9
Caelo	Tetracycline hydrochloride	17285808	8
Caelo	Tetracycline hydrochloride	17285809	5
Caelo	Tetracycline hydrochloride	1811031/01	1
Caelo	Tetracycline hydrochloride	1811031-01	2
Caelo	Tetracycline hydrochloride	18198602	8
Caelo	Tetracycline hydrochloride	18198603	9
Caelo	Tetracycline hydrochloride	18198604	2
Caelo	Tetracycline hydrochloride	18198608	12
Caelo	Tetracycline hydrochloride	18198612	4
Caelo	Tetracycline hydrochloride	18300213	1
Caelo	Tetracycline hydrochloride	18308302	4
Caelo	Tetracycline hydrochloride	18308303	2
Caelo	Tetracycline hydrochloride	18308305	12
Caelo	Tetracycline hydrochloride	18308306	2
Caelo	Tetracycline hydrochloride	18308313	4
Caelo	Tetracycline hydrochloride	18308314	3
Caelo	Tetracycline hydrochloride	192021003	11
Caelo	Tetracycline hydrochloride	192021004	11
Caelo	Tetracycline hydrochloride	192021008	4
Caelo	Tetracycline hydrochloride	192021011	26
Caelo	Tetracycline hydrochloride	1920221011	1
Caelo	Tetracycline hydrochloride	200003996008	1
Caelo	Tetracycline hydrochloride	20001708003	2
Caelo	Tetracycline hydrochloride	20001708004	8
Caelo	Tetracycline hydrochloride	20001708005	5
Caelo	Tetracycline hydrochloride	2000178003	1
Caelo	Tetracycline hydrochloride	20003996002	4
Caelo	Tetracycline hydrochloride	20003996003	9
Caelo	Tetracycline hydrochloride	20003996004	4
Caelo	Tetracycline hydrochloride	20003996006	6
Caelo	Tetracycline hydrochloride	20003996010	6
Caelo	Tetracycline hydrochloride	20003996011	4
Caelo	Tetracycline hydrochloride	20003996017	1
Caelo	Tetracycline hydrochloride	2000399606	1
Caelo	Tetracycline hydrochloride	21003348002	4
Caelo	Tetracycline hydrochloride	21003348003	7
Caelo	Tetracycline hydrochloride	21003348004	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tetracycline hydrochloride	21003348008	1
Caelo	Tetracycline hydrochloride	21003348011	9
Caelo	Tetracycline hydrochloride	21003348033	1
Caelo	Tetracycline hydrochloride	2714U-02378	1
Caelo	Tetracycline hydrochloride	2883	1
Caelo	Tetracycline hydrochloride	3314	1
Caelo	Tetracycline hydrochloride	3341	1
Caelo	Tetracycline hydrochloride	4012Q-02378	1
Caelo	Tetracycline hydrochloride	4117I-02378	1
Caelo	Tetracycline hydrochloride	4315I-02378	1
Caelo	Tetracycline hydrochloride	5091202	1
Caelo	Tetracycline hydrochloride	8682	1
Caelo	Tetracycline hydrochloride	9248704	1
Caesar & Lorenz GmbH	Tetracycline hydrochloride	18308312	1
Caesar & Lorenz GmbH	Tetracycline hydrochloride	20001708005	1
Caesar & Loretz GmbH...	Tetracycline hydrochloride	18308312	1
Caesar & Loretz GmbH...	Tetracycline hydrochloride	192021010	2
Caesar & Loretz GmbH...	Tetracycline hydrochloride	20001708005	1
Caesar & Loretz GmbH...	Tetracycline hydrochloride	20003996008	2
Caesar & Loretz GmbH...	Tetracycline hydrochloride	21003348004	2
Caesar & Loretz GmbH...	Tetracycline hydrochloride	18308306	1
Caesar & Loretz GmbH...	Tetracycline hydrochloride	21003348011	1
Caesar & Loretz GmbH /E	Tetracycline hydrochloride	18308305	1
Caesar & Loretz GmbH...	Tetracycline hydrochloride	20003996010	1
Caesar & Loretz GmbH...	Tetracycline hydrochloride	192021004	1
Caesar & Loretz GmbH...	Tetracycline hydrochloride	192021011	1
Caesar & Loretz GmbH...	Tetracycline hydrochloride	18308302	1
Caesar & Loretz GmbH/Kehr	Tetracycline hydrochloride	18198612	1
Caesar & Loretz GmbH...	Tetracycline hydrochloride	18308313	1
Caesar & Loretz GmbH/Phoe	Tetracycline hydrochloride	20003996004	1
Caesar & Loretz GmbH...	Tetracycline hydrochloride	20001708004	1
Caesar & Loretz GmbH	Tetracycline hydrochloride	102021011	1
Caesar & Loretz GmbH	Tetracycline hydrochloride	18198612	2
Caesar & Loretz GmbH	Tetracycline hydrochloride	18308302	1
Caesar & Loretz GmbH	Tetracycline hydrochloride	18308303	1
Caesar & Loretz GmbH	Tetracycline hydrochloride	18308305	2
Caesar & Loretz GmbH	Tetracycline hydrochloride	18308306	1
Caesar & Loretz GmbH	Tetracycline hydrochloride	18308313	2
Caesar & Loretz GmbH	Tetracycline hydrochloride	192021003	2
Caesar & Loretz GmbH	Tetracycline hydrochloride	192021008	2
Caesar & Loretz GmbH	Tetracycline hydrochloride	192021011	6
Caesar & Loretz GmbH	Tetracycline hydrochloride	20001708004	2
Caesar & Loretz GmbH	Tetracycline hydrochloride	20001708005	1
Caesar & Loretz GmbH	Tetracycline hydrochloride	20003996002	1
Caesar & Loretz GmbH	Tetracycline hydrochloride	20003996003	1
Caesar & Loretz GmbH	Tetracycline hydrochloride	20003996004	3
Caesar & Loretz GmbH	Tetracycline hydrochloride	20003996006	4
Caesar & Loretz GmbH	Tetracycline hydrochloride	20003996010	1
Caesar & Loretz GmbH	Tetracycline hydrochloride	20003996011	3
Caesar & Loretz GmbH	Tetracycline hydrochloride	20003996017	2
Caesar & Loretz GmbH	Tetracycline hydrochloride	21003348002	2
Caesar & Loretz GmbH	Tetracycline hydrochloride	21003348003	2
Caesar & Loretz GmbH	Tetracycline hydrochloride	21003348010	1
Caesar & Loretz GmbH	Tetracycline hydrochloride	21003348011	1
Caesar / Gehe	Tetracycline hydrochloride	16116706	1
Celo/Kehr	Tetracycline hydrochloride	13201307	1
EuRho / 107	Tetracycline hydrochloride	1811031-01	1
EuRho/AHD	Tetracycline hydrochloride		1
Eurho/Phoenix	Tetracycline hydrochloride	1204039-02	1
EuRho/Phoenix	Tetracycline hydrochloride	1811031-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho/Phoenix	Tetracycline hydrochloride	2004023-01	1
Eurho/Phönix	Tetracycline hydrochloride	1811031-01	2
EuRho/Sanacorp	Tetracycline hydrochloride	2004023-01	1
EuRho	Tetracycline hydrochloride	1302012-02	1
EuRho	Tetracycline hydrochloride	1402030-02	1
EuRho	Tetracycline hydrochloride	1811031-01	3
euRho	Tetracycline hydrochloride	2004023-01	1
EuRho	Tetracycline hydrochloride	2004023-01	1
EuRho	Tetracycline hydrochloride	2203017-01	1
Euro OTC	Tetracycline hydrochloride	100518-62	1
Euro OTC	Tetracycline hydrochloride	1103003-01	1
Euro OTC	Tetracycline hydrochloride	1110029-01	2
Euro OTC	Tetracycline hydrochloride	12040390	1
Euro OTC	Tetracycline hydrochloride	1204039-01	5
Euro OTC	Tetracycline hydrochloride	120403902	1
Euro OTC	Tetracycline hydrochloride	1204039-02	11
Euro OTC	Tetracycline hydrochloride	1302012-01	7
Euro OTC	Tetracycline hydrochloride	1302012-02	16
Euro OTC	Tetracycline hydrochloride	13042015C	1
Euro OTC	Tetracycline hydrochloride	140203001	1
Euro OTC	Tetracycline hydrochloride	1402030-01	9
Euro OTC	Tetracycline hydrochloride	1402030-02	9
Euro OTC	Tetracycline hydrochloride	140410-62	1
Euro OTC	Tetracycline hydrochloride	14120007-01	1
Euro OTC	Tetracycline hydrochloride	141200701	1
Euro OTC	Tetracycline hydrochloride	1412007-01	12
Euro OTC	Tetracycline hydrochloride	1412007-03	12
Euro OTC	Tetracycline hydrochloride	150601201	2
Euro OTC	Tetracycline hydrochloride	1506012-01	29
Euro OTC	Tetracycline hydrochloride	1506012-02	6
Euro OTC	Tetracycline hydrochloride	1506012-02Eur	1
Euro OTC	Tetracycline hydrochloride	151018-61	1
Euro OTC	Tetracycline hydrochloride	160302	1
Euro OTC	Tetracycline hydrochloride	1603026	2
Euro OTC	Tetracycline hydrochloride	1603026_01	1
Euro OTC	Tetracycline hydrochloride	160302601	1
Euro OTC	Tetracycline hydrochloride	1603026-01	42
Euro OTC	Tetracycline hydrochloride	16032026-01	1
Euro OTC	Tetracycline hydrochloride	160621TCH	1
Euro OTC	Tetracycline hydrochloride	1706020	2
Euro OTC	Tetracycline hydrochloride	170602001	4
Euro OTC	Tetracycline hydrochloride	1706020-01	66
Euro OTC	Tetracycline hydrochloride	1706020-02	2
Euro OTC	Tetracycline hydrochloride	17060201-01	1
Euro OTC	Tetracycline hydrochloride	180306T/1412007-03	1
Euro OTC	Tetracycline hydrochloride	1811031	2
Euro OTC	Tetracycline hydrochloride	181103101	1
Euro OTC	Tetracycline hydrochloride	1811031-01	81
Euro OTC	Tetracycline hydrochloride	1811031-02	4
Euro OTC	Tetracycline hydrochloride	18308314	1
Euro OTC	Tetracycline hydrochloride	20004023-01	1
Euro OTC	Tetracycline hydrochloride	2004023	3
Euro OTC	Tetracycline hydrochloride	200402301	3
Euro OTC	Tetracycline hydrochloride	2004023-01	54
Euro OTC	Tetracycline hydrochloride	2004023-02	5
Euro OTC	Tetracycline hydrochloride	210301501	1
Euro OTC	Tetracycline hydrochloride	2103015-01	11
Euro OTC	Tetracycline hydrochloride	2103015-02	1
Euro OTC	Tetracycline hydrochloride	21031702	1
Euro OTC	Tetracycline hydrochloride	21111404	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Tetracycline hydrochloride	22(1706020-01)	1
Euro OTC	Tetracycline hydrochloride	2203017-01	2
Euro OTC	Tetracycline hydrochloride	2301001	1
Euro OTC	Tetracycline hydrochloride	27101708	1
Euro OTC	Tetracycline hydrochloride	28021315	1
Euro OTC	Tetracycline hydrochloride	29052001	1
Euro OTC	Tetracycline hydrochloride	411682	1
Euro OTC	Tetracycline hydrochloride	80111031-01	1
Euro OTC	Tetracycline hydrochloride	RetestCharge20219/3	1
Euro OTG/ AHD	Tetracycline hydrochloride	1706020-01	1
EUro/AHD	Tetracycline hydrochloride	1302012-01	1
Euro/Anzag	Tetracycline hydrochloride	1603026-01	1
Euro/Jenne	Tetracycline hydrochloride	2004023-01	2
EuRo/Noweda	Tetracycline hydrochloride	1603026-01	1
EuRo/Noweda	Tetracycline hydrochloride	1706020-01	1
euro/phönix	Tetracycline hydrochloride	1506012-01	2
Euro/Phönix	Tetracycline hydrochloride	200402302	1
Euro/Sanacorp	Tetracycline hydrochloride	1811031-01	2
EuRoh/ Gehe	Tetracycline hydrochloride	1811031	1
Europh/An	Tetracycline hydrochloride	2004023-01	1
Europharm/Otto	Tetracycline hydrochloride	1204039-01	1
Europharm/Otto	Tetracycline hydrochloride	1204039-02	3
Fagron	Tetracycline hydrochloride	12E10-N015	1
Fagron	Tetracycline hydrochloride	12E10-N05	1
Fagron	Tetracycline hydrochloride	12J15-N05	1
Fagron	Tetracycline hydrochloride	13201301	1
Fagron	Tetracycline hydrochloride	13F17-N03	4
Fagron	Tetracycline hydrochloride	13J22-N04	1
Fagron	Tetracycline hydrochloride	13L10-B02-294454	1
Fagron	Tetracycline hydrochloride	13L10-B02-294455	2
Fagron	Tetracycline hydrochloride	1402030-02	2
Fagron	Tetracycline hydrochloride	14H06-B05	1
Fagron	Tetracycline hydrochloride	14H06-B05-299498	1
Fagron	Tetracycline hydrochloride	14H06-B05-303911	1
Fagron	Tetracycline hydrochloride	14H06-B05-303912	7
Fagron	Tetracycline hydrochloride	14H06-B05-311707	1
Fagron	Tetracycline hydrochloride	14H06-B05-314870	1
Fagron	Tetracycline hydrochloride	14H06-Bo5-303912	1
Fagron	Tetracycline hydrochloride	1506012-01	1
Fagron	Tetracycline hydrochloride	18308305	1
Fargon/Noweda	Tetracycline hydrochloride	1811031-01	1
Gatt-Koller	Tetracycline hydrochloride	1700729	1
Gehe Rostock	Tetracycline hydrochloride	192021010	1
Gehe	Tetracycline hydrochloride	1110029-01	1
Gehe	Tetracycline hydrochloride	15230703	1
Gehe	Tetracycline hydrochloride	16116706	1
Gehe	Tetracycline hydrochloride	1706020-01	1
Gehe	Tetracycline hydrochloride	18198603	1
GEHE	Tetracycline hydrochloride	18198612	1
Gehe	Tetracycline hydrochloride	2000178003	1
Gehe	Tetracycline hydrochloride	2004023-01	1
Gehe	Tetracycline hydrochloride	2103015-01	2
Gehe	Tetracycline hydrochloride	2103015-02	1
GEHE	Tetracycline hydrochloride	2203017-01	1
Hoff/ Noweda	Tetracycline hydrochloride	14364604	1
Ichthyol/Phönix	Tetracycline hydrochloride	1603026-01	1
Ichthyol-Gesellschaft	Tetracycline hydrochloride	1603026-01	1
Jenne	Tetracycline hydrochloride	1506012-02	1
Jenne	Tetracycline hydrochloride	18198602	1
Jenne	Tetracycline hydrochloride	21003348011	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Kehr.22.04.2020	Tetracycline hydrochloride	192021004	1
Ningxia / Caesar & L…	Tetracycline hydrochloride	17285801	1
Ningxia Qiyuan Pharm…	Tetracycline hydrochloride	21003348002	1
Ningxia Qiyuan Pharm…	Tetracycline hydrochloride	1811031-01	1
ningxia	Tetracycline hydrochloride	1412007-01	1
Ningxia	Tetracycline hydrochloride	1603026-01	3
Noweda	Tetracycline hydrochloride	13201307	1
Noweda	Tetracycline hydrochloride	1412007-03	1
Noweda	Tetracycline hydrochloride	1506012-01	1
Noweda	Tetracycline hydrochloride	17285801	1
Noweda	Tetracycline hydrochloride	17285802	1
Noweda	Tetracycline hydrochloride	18198603	1
Noweda	Tetracycline hydrochloride	21003348011	1
Noweda	Tetracycline hydrochloride	2203017-01	1
Noweda	Tetracycline hydrochloride	23000427003	2
Ph.Eur/Sanacorp	Tetracycline hydrochloride	1811031-01	1
Phoenix	Tetracycline hydrochloride	170602001	3
Phoenix	Tetracycline hydrochloride	18198612	1
Phoenix	Tetracycline hydrochloride	3428	1
Phönix Gotha	Tetracycline hydrochloride	1302012-01	1
Phönix	Tetracycline hydrochloride	16116715	1
PHÖNIX	Tetracycline hydrochloride	16116721	1
Phönix	Tetracycline hydrochloride	1706020-01	1
PHÖNIX	Tetracycline hydrochloride	192021004	1
phönix	Tetracycline hydrochloride	2103015-01	1
phönix	Tetracycline hydrochloride	2203017-01	1
Röntgen	Tetracycline hydrochloride	17285801	1
s. Protokol	Tetracycline hydrochloride		1
Sanacorp	Tetracycline hydrochloride	100403401	1
Sanacorp	Tetracycline hydrochloride	1402030-01	1
Sanacorp	Tetracycline hydrochloride	1603026-01	1
Sanacorp	Tetracycline hydrochloride	192021011	1
Sanacorp	Tetracycline hydrochloride	204023-01	1
Sanacorp	Tetracycline hydrochloride	21003348008	1
Sanacorp	Tetracycline hydrochloride	2203017-01	1
yinchuan Ningxia	Tetracycline hydrochloride	1811031-01	1

- 235 035 spectra from 1515 *Apo-Ident* customers from a total of 49 074 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tetracycline hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tetracycline hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	460	0	152 502
Type B	0	320	0	201 764
Type C	0	1027	5	235 035

The substance/substance group *Tetracycline hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6957 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.1250 %)
Type C	100.0000 % (> 99.9007 %)	99.5155 % (> 99.2248 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21079	21079	0.00	153.72
21427	21835	11.79	122.81
21428	21835	8.49	110.59
21835	21835	0.00	95.75
22468	22468	0.00	244.54
22833	25686	8.96	170.86
25279	25279	0.00	189.61
25686	25686	0.00	156.09
26301	21079	8.09	152.48

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Theophylline**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20723-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Theophylline; Theophyllinum

Special notes

When selecting the *Theophylline* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Theophylline	6	3	13

Second-stage model

For differentiation of the substance/substance group *Theophylline* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Theophylline* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Midazolam hydrochloride	112.26	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Theophylline* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Theophylline*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Theophylline	12166316	20723	40	1402055
Caelo	Theophylline	12341101	21740	60	20121115
Caelo	Theophylline	192563	24902	40	20191120*
Caelo	Theophylline	22001229002	26236	40	20220505
Caelo	Theophylline	24001902	27317	40	20240819*
Gatt-Koller	Theophylline	23J01412	27095	30	20230809

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 250 spectra of 6 reference samples from the substance/substance group *Theophylline*. These

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 712 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 180 spectra of 6 reference samples from the substance/substance group *Theophylline*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Theophylline	15203018	23253	40
Caelo	Theophylline	171962	23854	40
Caelo	Theophylline	23001176	26838	40
Caelo	Theophylline	22001229002	26236SI†	20
Caelo	Theophylline	23001176	26838SI	20
Gatt-Koller	Theophylline	23J01412	27095SI†	20

- 201 904 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 24 spectra from 21 *Apo-Ident* customers from 15 batches from the substance/substance group *Theophylline*.
- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Theophylline	22001229009	1
Alliance Healthcare	Theophylline	192563003	1
Caelo	Theophylline	12166305	2
Caelo	Theophylline	12166306	1
Caelo	Theophylline	12166311	1
Caelo	Theophylline	12166312	3
Caelo	Theophylline	12166315	1
Caelo	Theophylline	12341101	2
Caelo	Theophylline	12341104	1
Caelo	Theophylline	15203010	1
Caelo	Theophylline	17196203	2
Caelo	Theophylline	18097508	1
Caelo	Theophylline	22001229002	1
Caelo	Theophylline	22001229006	1
Caesar & Loretz GmbH	Theophylline	21000106001	1
Caesar & Loretz GmbH	Theophylline	22001229002	1
Caesar&loretz,Phoenix	Theophylline	12166315	1
Caeser und Loretz GmbH	Theophylline	18097508	1
Noweda	Theophylline	12166305	1

- 236 043 spectra from 1515 *Apo-Ident* customers from a total of 49 243 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Theophylline* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Theophylline* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	250	0	152 712
Type B	0	180	0	201 904
Type C	0	24	0	236 043

The substance/substance group *Theophylline* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.6000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.6667 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 75.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20723	20723	0.00	254.97
21740	20723	16.47	269.15
24902	24902	0.00	253.95
26236	24902	7.77	253.10
27095	20723	13.45	243.80
27317	27317	0.00	248.08

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Theophylline-ethylenediamine hydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20831-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Theophylline-ethylenediamine hydrate; Theophyllinum et ethylendiaminum hydricum

Special notes

When selecting the *Theophylline-ethylenediamine hydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Theophylline-ethylenediamine hydrate	7	5	2

Second-stage model

For differentiation of the substance/substance group *Theophylline-ethylenediamine hydrate* the following second-stage model is used:

- Submodel 12

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Theophylline-ethylenediamine hydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Glycine	106.12	–
⋮	⋮	⋮
Clioquinol	>50	20.49
Mesalazine	>50	46.19
Miconazole nitrate	>50	49.72
Nicotinic acid	>50	112.58

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Theophylline-ethylenediamine hydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Theophylline-ethylenediamine hydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Theophylline-ethylenediam…	12145301	20831	40	20120628
Caelo	Theophylline-ethylenediam…	12363708	20992	40	20130116
Caelo	Theophylline-ethylenediam…	13268609	21549	40	1412133
Caelo	Theophylline-ethylenediam…	15380302	22589	40	20160211
Caelo	Theophylline-ethylenediam…	17073707	23564	30	20170323
Caelo	Theophylline-ethylenediam…	192220	24903	40	20191204*
Caelo	Theophylline-ethylenediam…	20004052	25510	40	20201201

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 270 spectra of 7 reference samples from the substance/substance group *Theophylline-ethylenediamine hydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 692 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 250 spectra of 8 reference samples from the substance/substance group *Theophylline-ethylenediamine hydrate*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Theophylline-ethylenediam…	172999	23823	40
Caelo	Theophylline-ethylenediam…	182738	24383	40
Caelo	Theophylline-ethylenediam…	22000118006	25974	40
Caelo	Theophylline-ethylenediam…	22003464	26499	40
Caelo	Theophylline-ethylenediam…	23003143	27237	40
Caelo	Theophylline-ethylenediam…	22000118006	25974SI	10
Caelo	Theophylline-ethylenediam…	22003464	26499SI	20
Caelo	Theophylline-ethylenediam…	23003143	27237SI	20

- 201 834 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 4 spectra from 4 *Apo-Ident* customers from 3 batches from the substance/substance group *Theophylline-ethylenediamine hydrate*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
ACM / Phoenix	Theophylline-ethylenediam…	KNC0896J14	1
Caelo	Theophylline-ethylenediam…	15380302	1
Caelo	Theophylline-ethylenediam…	20003320003	1
Caesar & Loretz GmbH	Theophylline-ethylenediam…	20003320003	1

- 236 063 spectra from 1515 *Apo-Ident* customers from a total of 49 255 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Theophylline-ethylenediamine hydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Theophylline-ethylenediamine hydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	270	0	152 692
Type B	0	250	0	201 834
Type C	0	4	0	236 063

The substance/substance group *Theophylline-ethylenediamine hydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.7778 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.6000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20831	21549	9.61	153.64
20992	21549	5.56	152.40
21549	21549	0.00	150.97
22589	24903	7.59	157.99
23564	24903	9.72	161.06
24903	24903	0.00	156.83
25510	21549	14.40	158.76

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Thiamine chloride hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20566-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Thiamine chloride hydrochloride; Thiamini hydrochloridum

Special notes

When selecting the *Thiamine chloride hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Thiamine chloride hydrochloride	9	11	38

Second-stage model

For differentiation of the substance/substance group *Thiamine chloride hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Thiamine chloride hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	88.79	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Thiamine chloride hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Thiamine chloride hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Thiamine chloride hydroch…	14069502	21478	60	20140321
Caelo	Thiamine chloride hydroch…	14069502	21511	60	8986
Caelo	Thiamine chloride hydroch…	160156	22477	60	20160316*
Caelo	Thiamine chloride hydroch…	192567	25095	40	20191216*
Caelo	Thiamine chloride hydroch…	20001173	25193	40	20200724*
Euro OTC	Thiamine chloride hydroch…	1211008-02	21647	60	20121122
Euro OTC	Thiamine chloride hydroch…	1612004	22919	40	20170117*
Euro OTC	Thiamine chloride hydroch…	2004007	25274	40	20200618*
Euro OTC	Thiamine chloride hydroch…	2007034	25332	40	20200909*
Euro OTC	Thiamine chloride hydroch…	2309008	26928	40	20231006*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 480 spectra of 10 reference samples from the substance/substance group *Thiamine chloride hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 482 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 475 spectra of 14 reference samples from the substance/substance group *Thiamine chloride hydrochloride*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Thiamine chloride hydroch…	170976	23368	40
Caelo	Thiamine chloride hydroch…	21002868002	26416	30
Caelo	Thiamine chloride hydroch…	22003533	26482	40
Caelo	Thiamine chloride hydroch…	23001172	26835	40
Euro OTC	Thiamine chloride hydroch…	1705034	23439	40
Euro OTC	Thiamine chloride hydroch…	1712013	23911	40
Euro OTC	Thiamine chloride hydroch…	1807001	24146	40
Euro OTC	Thiamine chloride hydroch…	2201045	25961	40
Euro OTC	Thiamine chloride hydroch…	2207008	26211	40
Fagron	Thiamine chloride hydroch…	22I22-B05-223757	26536	40
Fagron	Thiamine chloride hydroch…	23G04-B12-239937	27191	40
Caelo	Thiamine chloride hydroch…	22003533	26482SI	20
Euro OTC	Thiamine chloride hydroch…	2201045	25961SI	5
Euro OTC	Thiamine chloride hydroch…	2207008	26211SI	20

- 201 609 spectra from a total of 4034 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 62 spectra from 28 *Apo-Ident* customers from 40 batches from the substance/substance group *Thiamine chloride hydrochloride*.

- Among them are spectra of independent samples from 38 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Thiamine chloride hydroch…		1
Caelo	Thiamine chloride hydroch…	11061401	1
Caelo	Thiamine chloride hydroch…	11371309	2
Caelo	Thiamine chloride hydroch…	11371313	1
Caelo	Thiamine chloride hydroch…	11371319	3
Caelo	Thiamine chloride hydroch…	12091407	1
Caelo	Thiamine chloride hydroch…	12340712	1
Caelo	Thiamine chloride hydroch…	13296610	4
Caelo	Thiamine chloride hydroch…	14069502	1
Caelo	Thiamine chloride hydroch…	15003201	1
Caelo	Thiamine chloride hydroch…	15199009	2
Caelo	Thiamine chloride hydroch…	15199099	1
Caelo	Thiamine chloride hydroch…	15269613	1
Caelo	Thiamine chloride hydroch…	16015607	1
Caelo	Thiamine chloride hydroch…	16015609	1
Caelo	Thiamine chloride hydroch…	17097602	1
Caelo	Thiamine chloride hydroch…	171201301	1
Caelo	Thiamine chloride hydroch…	18163717	2
Caelo	Thiamine chloride hydroch…	20001173002	2
Caelo	Thiamine chloride hydroch…	20004527005	1
Caelo	Thiamine chloride hydroch…	4071402	1
Caelo	Thiamine chloride hydroch…	5122	1
Caelo	Thiamine chloride hydroch…	8121405	1
Caesar & Loretz GmbH	Thiamine chloride hydroch…	18163705	1
Caesar & Loretz GmbH	Thiamine chloride hydroch…	18163709	2
Caesar & Loretz GmbH	Thiamine chloride hydroch…	18163717	1
Caesar & Loretz GmbH	Thiamine chloride hydroch…	20004527005	5
Euro OTC	Thiamine chloride hydroch…	1211008-01	1
Euro OTC	Thiamine chloride hydroch…	161200401	1
Euro OTC	Thiamine chloride hydroch…	1705034-01	2
Euro OTC	Thiamine chloride hydroch…	1712013-01	1
Euro OTC	Thiamine chloride hydroch…	1807001-01	3
Euro OTC	Thiamine chloride hydroch…	2004007-01	1
Euro OTC	Thiamine chloride hydroch…	2007034-01	1
Euro OTC	Thiamine chloride hydroch…	2207008-01	1
Fagron	Thiamine chloride hydroch…	10111401	1
Fagron	Thiamine chloride hydroch…	13E22-No8	1
Fagron	Thiamine chloride hydroch…	17F23-B02-340810	1
Fagron	Thiamine chloride hydroch…	190115006	1
Fagron	Thiamine chloride hydroch…	20A13-B08-196821	1
Fagron	Thiamine chloride hydroch…	20F16-B09-201351	2
Finze	Thiamine chloride hydroch…	9216114	1
Jiangxi Tianxin	Thiamine chloride hydroch…	1807001-01	1
Sanacorp	Thiamine chloride hydroch…	12340712	1

- 236 005 spectra from 1515 *Apo-Ident* customers from a total of 49 219 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Thiamine chloride hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Thiamine chloride hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	480	0	152 482
Type B	0	475	0	201 609
Type C	0	62	0	236 005

The substance/substance group *Thiamine chloride hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.7368 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 90.3226 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21478	25274	11.78	173.85
21511	21511	0.00	181.83
21647	22477	10.49	191.24
22477	22477	0.00	201.46
22919	22919	0.00	181.19
25095	25095	0.00	180.33
25193	25193	0.00	186.43
25274	25274	0.00	177.26
25332	25332	0.00	169.43
26928	26928	0.00	159.81

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Thiomersal**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20702-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Thiomersal; Thiomersalum

Special notes

When selecting the *Thiomersal* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Thiomersal	3	1	13

Second-stage model

For differentiation of the substance/substance group *Thiomersal* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Thiomersal* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prilocaine hydrochloride	98.29	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Thiomersal* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Thiomersal*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Thiomersal	172173	23679	30	20170919*
Caelo	Thiomersal	22003780	27219	40	20230404*
Caelo	Thiomersal	22003780	27219SI	20	20230404*
Fagron	Thiomersal	11K01-N03	20702	40	1401417

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 130 spectra of 4 reference samples from the substance/substance group *Thiomersal*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 832 spectra from a total of 2839 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Thiomersal*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Thiomersal	193090	25198	40

- 202 044 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 17 spectra from 13 *Apo-Ident* customers from 14 batches from the substance/substance group *Thiomersal*.
- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Thiomersal	22003780001	1
	Thiomersal	22003780002	1
	Thiomersal	23003535001	2
Caelo	Thiomersal	10296413	1
Caelo	Thiomersal	13577020	1
Caelo	Thiomersal	20004306001	1
Caelo	Thiomersal	20004306002	1
Caelo	Thiomersal	20004306003	2
Caelo	Thiomersal	21051507	1
Caesar & Loretz GmbH	Thiomersal	12275218	1
Caesar & Loretz GmbH	Thiomersal	193090002	1
Caesar & Loretz GmbH	Thiomersal	20004306003	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Thiomersal		1
Fagron	Thiomersal	12F19-N11	1
Fagron	Thiomersal	12J17-N02	1

- 236 050 spectra from 1515 *Apo-Ident* customers from a total of 49 244 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Thiomersal* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Thiomersal* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	130	0	152 832
Type B	0	40	0	202 044
Type C	0	17	0	236 050

The substance/substance group *Thiomersal* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.3846 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20702	20702	0.00	134.87
23679	23679	0.00	140.08
27219	27219	0.00	133.94

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Thymol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20003-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Thymol; Thymolum

Special notes

When selecting the *Thymol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Thymol	8	9	79

Second-stage model

For differentiation of the substance/substance group *Thymol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Thymol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Menthol	79.70	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Thymol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Thymol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Thymol	14025805	21469	60	20140127
Caelo	Thymol	16144101	23160	40	20160606
Caelo	Thymol	173407	23837	40	20180110*
Caelo	Thymol	21000880	25650	40	20210401*
Caelo	Thymol	23001568	26840	40	20230622*
Caelo	Thymol	23001568	26840SI	40	20230622*
Euro OTC	Thymol	1312022-02	21639	60	20131219
Euro OTC	Thymol	1510004	21943	60	20151016*
Fagron	Thymol	15H13-B05-328912	23499	40	20151118

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 420 spectra of 9 reference samples from the substance/substance group *Thymol*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 542 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 409 spectra of 11 reference samples from the substance/substance group *Thymol*.

- Among them are spectra of independent samples from 9 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Thymol	181424	24231	40
Caelo	Thymol	190342	24552	40
Caelo	Thymol	21002863	25862	50
Caelo	Thymol	22002344	26245	40
Caelo	Thymol	22002044	26258	40
Caelo	Thymol	24000390	27122	40
Caelo	Thymol	24001437	27313	39
Euro OTC	Thymol	1710037	23773	40
Euro OTC	Thymol	1808014	24299	40
Caelo	Thymol	22002344	26245SI	20
Caelo	Thymol	22002044	26258SI	20

- 201 675 spectra from a total of 4036 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 234 spectra from 180 *Apo-Ident* customers from 82 batches from the substance/substance group *Thymol*.

- Among them are spectra of independent samples from 79 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Thymol	14025802	1
	Thymol	22002044004	1
	Thymol	23000600003	1
ACM / Herba	Thymol	KNC1166J14	1
Alliance Healthcare	Thymol	20003672009	1
apo-ident	Thymol	1808014-01	1
Caelo	Thymol	11178718	1
Caelo	Thymol	11358607	2
Caelo	Thymol	11358608	1
Caelo	Thymol	11358616	2
Caelo	Thymol	13147502	2
Caelo	Thymol	13288802	4
Caelo	Thymol	13288806	1
Caelo	Thymol	14025802	2
Caelo	Thymol	14025805	1
Caelo	Thymol	14025807	1
Caelo	Thymol	14025809	2
Caelo	Thymol	14025815	1
Caelo	Thymol	14025816	1
Caelo	Thymol	14302401	1
Caelo	Thymol	14310601	2
Caelo	Thymol	14310605	1
Caelo	Thymol	15130101	2
Caelo	Thymol	15130106	3
Caelo	Thymol	15362901	5
Caelo	Thymol	15362908	4
Caelo	Thymol	16144101	6
Caelo	Thymol	16144105	7
Caelo	Thymol	16144108	7
Caelo	Thymol	161441108	1
Caelo	Thymol	1730711	1
Caelo	Thymol	17324203	4
Caelo	Thymol	17340708	1
Caelo	Thymol	17340711	7
Caelo	Thymol	17340716	2
Caelo	Thymol	18221907	1
Caelo	Thymol	19034203	5
Caelo	Thymol	19034205	4
Caelo	Thymol	19061303	1
Caelo	Thymol	192437003	3
Caelo	Thymol	19243701	9
Caelo	Thymol	20001482001	6
Caelo	Thymol	20001482003	5
Caelo	Thymol	20003672003	3
Caelo	Thymol	20003672006	6
Caelo	Thymol	20003672007	5
Caelo	Thymol	20003750002	1
Caelo	Thymol	2031503	1
Caelo	Thymol	21000880002	2
Caelo	Thymol	21000880007	2
Caelo	Thymol	2100088002	1
Caelo	Thymol	21042	1
Caelo	Thymol	4364887223	1
Caesar & Loretz GmbH...	Thymol	19034205	1
Caesar & Loretz GmbH...	Thymol	21000880009	1
Caesar & Loretz GmbH...	Thymol	19034203	1
Caesar & Loretz GmbH...	Thymol	192437003	1
Caesar & Loretz GmbH...	Thymol	18221907	1
Caesar & Loretz GmbH...	Thymol	20003672009	1
Caesar & Loretz GmbH	Thymol	16144101	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Thymol	17340711	1
Caesar & Loretz GmbH	Thymol	17340716	2
Caesar & Loretz GmbH	Thymol	19034203	1
Caesar & Loretz GmbH	Thymol	19034205	1
Caesar & Loretz GmbH	Thymol	192437003	1
Caesar & Loretz GmbH	Thymol	19243701	3
Caesar & Loretz GmbH	Thymol	20001482001	2
Caesar & Loretz GmbH	Thymol	20003672003	3
Caesar & Loretz GmbH	Thymol	20003672006	2
Caesar & Loretz GmbH	Thymol	20003672007	2
Caesar & Loretz GmbH	Thymol	20003750002	1
Caesar & Loretz GmbH	Thymol	21000880005	1
Caesar & Loretz GmbH	Thymol	21000880007	1
Caesar § Lorenz GmbH	Thymol	13288806	1
Ebert & Jacobi 02...	Thymol	15362901	1
Euro OTC	Thymol	1107021-01	1
Euro OTC	Thymol	11358603	1
Euro OTC	Thymol	1202028-01	1
Euro OTC	Thymol	1312022-01	1
Euro OTC	Thymol	1410007-01	5
Euro OTC	Thymol	15100004-03	1
Euro OTC	Thymol	1510004-01	2
Euro OTC	Thymol	1510004-02	9
Euro OTC	Thymol	1510004-03	1
Euro OTC	Thymol	1710037-01	5
Euro OTC	Thymol	1808014-01	3
Euro OTC	Thymol	20151012-1	1
Euro/ Phönix	Thymol	1510004-02	1
Euro/Phönix	Thymol	180801401	1
Fagron	Thymol	12B06-N11	1
Fagron	Thymol	12E30-N11	1
Fagron	Thymol	12H29-N02	2
Fagron	Thymol	12K01-N02	2
Fagron	Thymol	12M29-N02	1
Fagron	Thymol	713575	1
Fagron	Thymol	8G23-N09	2
Frey+Lau GmbH/Phönix	Thymol	1312022-01	1
Gehe Kassel	Thymol	1312022-01	1
gehe	Thymol	1808014-01	1
Gehe	Thymol	19243701	1
gehe	Thymol	20003672003	1
gehe	Thymol	5112139	1
L12	Thymol	15172002	1
L30	Thymol	1510004-03	1
Noweda	Thymol	12k01-no2	1
Noweda	Thymol	16144105	1
Noweda	Thymol	20003750007	2
PHOENIX 26.03.2014	Thymol	14025802	2
Phoenix	Thymol	19034205	1
Phoenix	Thymol	20001482003	1
Phönix	Thymol	11358610	1
Phönix	Thymol	1510004-01	1
Phönix	Thymol	20001482003	1
Sanacorp	Thymol	1135816	1
Sanacorp	Thymol	9E14-N16	1
xxxxx	Thymol		1
xxxxx	Thymol	RT1211	1

- 235 833 spectra from 1515 *Apo-Ident* customers from a total of 49 177 batches from a further

721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Thymol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Thymol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	420	0	152 542
Type B	0	409	0	201 675
Type C	0	234	0	235 833

The substance/substance group *Thymol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5714 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.5330 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 97.4359 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21469	23837	13.96	123.17
21639	23837	10.94	122.78
21943	21943	0.00	127.80
23160	23837	17.58	122.64
23499	23837	7.33	124.42
23837	23837	0.00	123.41
25650	25650	0.00	122.63
26840	26840	0.00	118.32

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tobramycin sulfate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20951-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tobramycin sulfate; Tobramycin sulphate; Tobramycini sulfas

Special notes

When selecting the *Tobramycin sulfate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tobramycin sulfate	15	4	19

Second-stage model

For differentiation of the substance/substance group *Tobramycin sulfate* the following second-stage model is used:

- Submodel 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tobramycin sulfate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Neomycin sulfate	20.71	15.61
Polymyxin B sulfate	52.33	–
⋮	⋮	⋮
Riboflavin sodium phosphate hydrate	>50	69.59
Mg-Ca-K colamine phosphate	>50	75.74
Zinc gluconate	>50	87.49
Carbomers	>50	109.21
Gentamicin sulfate	>50	127.63
Magnesium citrate	>50	134.93
Sodium tetraborate	>50	473.95
Finasteride	>50	1421.13

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tobramycin sulfate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tobramycin sulfate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Tobramycin sulfate	AP15061047002T	22393	40	1608462
Audor Pharma	Tobramycin sulfate	AP15061047002T	23502	40	20160322
Euro OTC	Tobramycin sulfate	1301011-02	21624	60	1508071
Euro OTC	Tobramycin sulfate	1505015-01	21832	60	8963
Euro OTC	Tobramycin sulfate	1510035-01	22240	60	9202
Euro OTC	Tobramycin sulfate	1510035	22252	60	20151208*
Euro OTC	Tobramycin sulfate	1807045	24321	40	20180917*
Euro OTC	Tobramycin sulfate	2001010	25100	40	20200113*
Euro OTC	Tobramycin sulfate	2202013	26045	40	20220324*
Euro OTC	Tobramycin sulfate	2404002	27371	40	20240904*
Fagron	Tobramycin sulfate	12G03-N03	20951	40	1404541

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Tobramycin sulfate	15I17-B04-315697	22359	45	20150928
Fagron	Tobramycin sulfate	16B05-B03-336397	23515	40	1801385
Fagron	Tobramycin sulfate	20H13-F05-373631	25506	40	2105375
Fagron	Tobramycin sulfate	20F18-F05-376114	25507	40	2105376
Fagron	Tobramycin sulfate	23K07-B16-233773	27050	40	20231215
Fagron	Tobramycin sulfate	23K07-B16-233773	27050SI	20	20231215

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 745 spectra of 17 reference samples from the substance/substance group *Tobramycin sulfate*. These samples are listed above in the *calibration samples* section. The reference samples come from 15 different batches.

- 152 217 spectra from a total of 2827 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 190 spectra of 6 reference samples from the substance/substance group *Tobramycin sulfate*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Tobramycin sulfate	1710029	23870	40
Euro OTC	Tobramycin sulfate	1910008	25085	40
Euro OTC	Tobramycin sulfate	2211003	26569	40
Fagron	Tobramycin sulfate	20A14-F02-368920	25184	40
Euro OTC	Tobramycin sulfate	2202013	26045SI†	10
Euro OTC	Tobramycin sulfate	2211003	26569SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 894 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 33 spectra from 14 *Apo-Ident* customers from 22 batches from the substance/substance group *Tobramycin sulfate*.
- Among them are spectra of independent samples from 19 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tobramycin sulfate	22E06-B02-224488	2
	Tobramycin sulfate	B02-2283406	1
EuRho/VDL01	Tobramycin sulfate	1710029-01	1
Euro OCT/Noweda	Tobramycin sulfate	1510035-01	1
Euro OTC	Tobramycin sulfate	1505015-01	1
Euro OTC	Tobramycin sulfate	15I17-B04-315697	1
Euro OTC	Tobramycin sulfate	1807045-01	3
Fagron	Tobramycin sulfate	13H09-N09	1
Fagron	Tobramycin sulfate	15/17-B04-315697	1
Fagron	Tobramycin sulfate	16b-03-319433	1
Fagron	Tobramycin sulfate	16B05-B03	4
Fagron	Tobramycin sulfate	16B05-B03-317988	2
Fagron	Tobramycin sulfate	16B05-B03-319433	1
Fagron	Tobramycin sulfate	16B05-B03-330974	2
Fagron	Tobramycin sulfate	17E05-B03-338122	2
Fagron	Tobramycin sulfate	17J12-B04-341324	2
Fagron	Tobramycin sulfate	20A14-F02-368920	2
Fagron	Tobramycin sulfate	20H13-F05-373633	1
Fagron	Tobramycin sulfate	21A04-F02	1
Fagron	Tobramycin sulfate	21H30-B02-213664	1
Fagron	Tobramycin sulfate	21H30-B02-213666	1
PHOENIX 31.01.2014	Tobramycin sulfate	1202006-01	1

- 236 034 spectra from 1515 *Apo-Ident* customers from a total of 49 236 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tobramycin sulfate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tobramycin sulfate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	False positive	True positive	False negative	True negative
Type A	0	745	0	152 217
Type B	0	190	0	201 894
Type C	0	32	1	236 034

The substance/substance group *Tobramycin sulfate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1946 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.8421 %)
Type C	100.0000 % (> 99.9007 %)	96.9697 % (> 87.8788 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20951	20951	0.00	112.32
21624	21624	0.00	95.71
21832	21832	0.00	89.63
22240	22240	0.00	121.91
22252	22252	0.00	89.69
22359	23515	20.29	102.22
22393	22393	0.00	55.55
23502	25100	15.64	69.86
23515	23515	0.00	99.21
24321	24321	0.00	70.01
25100	25100	0.00	84.36
25506	25506	0.00	173.42
25507	25507	0.00	164.12
26045	26045	0.00	105.60
27050	22240	33.45	159.61
27371	27371	0.00	54.59

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tosylchloramide sodium**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20133-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tosylchloramide sodium; Tosylchloramidum natricum

Special notes

When selecting the *Tosylchloramide sodium* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tosylchloramide sodium	4	3	36

Second-stage model

For differentiation of the substance/substance group *Tosylchloramide sodium* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tosylchloramide sodium* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	67.09	–
⋮	⋮	⋮
Riboflavin	>50	26.67
Polymyxin B sulfate	>50	53.63
Hyoscine hydrobromide	>50	62.39
Bacitracin	>50	68.00
Cyanocobalamin	>50	69.16
Colistin sulfate	>50	71.78
Amphotericin B	>50	90.29
Calcium pantothenate	>50	103.14
Estradiol hemihydrate	>50	124.25
Nystatin	>50	124.33
Calcium glycerophosphate	>50	133.41
Triamcinolone	>50	144.65
Estriol	>50	157.90
SyrSpend® SF pH4 neo (Maize starch)	>50	178.05
alpha-tocopheryl acetate dry concentrate	>50	178.13
Methylcobalamin	>50	180.89
Selenium yeast	>50	196.45
Oxalic acid	>50	202.95
Gelatine, white	>50	203.25
SyrSpend® SF Alka	>50	205.50
Rice starch	>50	222.79
Carmellose sodium	>50	272.25
Wheat starch	>50	291.07
Fructose	>50	308.09
SyrSpend® SF pH4	>50	318.73
Potato starch	>50	341.64
Corn starch	>50	387.86
Acacia, dried dispersion	>50	399.91
Maltodextrin	>50	431.45

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tosylchloramide sodium* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tosylchloramide sodium*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Tosylchloramide sodium	13103201	20864	40	20130424
Caelo	Tosylchloramide sodium	13361602	21115	40	1407634
Caelo	Tosylchloramide sodium	16236603	23562	40	20160819
Caelo	Tosylchloramide sodium	172265	24238	40	20170906*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 160 spectra of 4 reference samples from the substance/substance group *Tosylchloramide sodium*. These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.
- 152 802 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 160 spectra of 4 reference samples from the substance/substance group *Tosylchloramide sodium*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Tosylchloramide sodium	13361606	21480	60
Caelo	Tosylchloramide sodium	162366	22773	40
Caelo	Tosylchloramide sodium	23000577	27114	40
Caelo	Tosylchloramide sodium	23000577	27114SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 924 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 93 spectra from 58 *Apo-Ident* customers from 37 batches from the substance/substance group *Tosylchloramide sodium*.

- Among them are spectra of independent samples from 36 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tosylchloramide sodium	89539524	1
Anzag	Tosylchloramide sodium	12H09-N01	1
Caelo	Tosylchloramide sodium	11116708	1
Caelo	Tosylchloramide sodium	12277005	3
Caelo	Tosylchloramide sodium	12323605	1
Caelo	Tosylchloramide sodium	12323606	1
Caelo	Tosylchloramide sodium	12323607	1
Caelo	Tosylchloramide sodium	12323609	2
Caelo	Tosylchloramide sodium	1310206	1
Caelo	Tosylchloramide sodium	13103206	8
Caelo	Tosylchloramide sodium	13103207	1
Caelo	Tosylchloramide sodium	13103210	2
Caelo	Tosylchloramide sodium	13361606	4
Caelo	Tosylchloramide sodium	13361607	6
Caelo	Tosylchloramide sodium	14183504	1
Caelo	Tosylchloramide sodium	14183509	1
Caelo	Tosylchloramide sodium	15039603	4
Caelo	Tosylchloramide sodium	15183905	1
Caelo	Tosylchloramide sodium	15370501	5
Caelo	Tosylchloramide sodium	15370505	2
Caelo	Tosylchloramide sodium	16236603	11
Caelo	Tosylchloramide sodium	16236603/1180117	1
Caelo	Tosylchloramide sodium	16236607	6
Caelo	Tosylchloramide sodium	16236611	3
Caelo	Tosylchloramide sodium	17061503	3
Caelo	Tosylchloramide sodium	17061511	1
Caelo	Tosylchloramide sodium	17226502	2
Caelo	Tosylchloramide sodium	17226503	4
Caelo	Tosylchloramide sodium	71051187	2
Caelo	Tosylchloramide sodium	72215377	2
Caeolo	Tosylchloramide sodium	16236607	1
EuRho	Tosylchloramide sodium	133610607	1
Fagron	Tosylchloramide sodium	11L08-N04	1
Fagron	Tosylchloramide sodium	14B27-B03-291967	1
Fagron	Tosylchloramide sodium	14L12-B01-301915	1
Hydra International Ltd	Tosylchloramide sodium	91020132	1
L10	Tosylchloramide sodium	16236607	2
Lysoform	Tosylchloramide sodium	K-09-2019	1
Sanacorp	Tosylchloramide sodium	12H09-N01	1
Taoasis	Tosylchloramide sodium	1623607	1

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 235 974 spectra from 1515 *Apo-Ident* customers from a total of 49 222 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tosylchloramide sodium* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tosylchloramide sodium* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	160	0	152 802
Type B	0	160	0	201 924
Type C	0	93	0	235 974

The substance/substance group *Tosylchloramide sodium* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 96.2500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 96.2500 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 93.5484 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20864	21115	21.06	152.61
21115	21115	0.00	144.74
23562	21115	16.88	150.77
24238	24238	0.00	151.76

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances,

thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tranexamic acid**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20397-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tranexamic acid; Acidum tranexamicum

Special notes

When selecting the *Tranexamic acid* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tranexamic acid	9	4	43

Second-stage model

For differentiation of the substance/substance group *Tranexamic acid* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tranexamic acid* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	83.84	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tranexamic acid* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tranexamic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Tranexamic acid	APX1508016MT	23504	40	20170224
Audor Pharma	Tranexamic acid	APX1803027MT	24708	40	20180430
Euro OTC	Tranexamic acid	2002005	25078	40	20200219*
Euro OTC	Tranexamic acid	2001034	25099	40	20200218*
Euro OTC	Tranexamic acid	2304017	26652	40	20230508*
Euro OTC	Tranexamic acid	2304017	26652SI	20	20230508*
Euro OTC	Tranexamic acid	2312001	27140	40	20240313*
Euro OTC	Tranexamic acid	2312001	27140SI	20	20240313*
Fagron	Tranexamic acid	14C21-B08-292225	21654	60	AR-17-FG-016394-01
Fagron	Tranexamic acid	14L15-B06-3000036	21727	60	AR-15-FG-008937-02
Fagron	Tranexamic acid	20H24-F02-373687	25586	40	20200923

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 440 spectra of 11 reference samples from the substance/substance group *Tranexamic acid*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 522 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 240 spectra of 6 reference samples from the substance/substance group *Tranexamic acid*.

- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Tranexamic acid	2006030	25247	40
Euro OTC	Tranexamic acid	2203031	26098	40
Fagron	Tranexamic acid	16E31-B07-331591	23503	50
Fagron	Tranexamic acid	21B05-F03-377271	25745	50
Euro OTC	Tranexamic acid	2203031	26098SI	20
Fagron	Tranexamic acid	16E31-B07-331591	23505	40

- 201 844 spectra from a total of 4041 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 102 spectra from 70 *Apo-Ident* customers from 49 batches from the substance/substance group *Tranexamic acid*.

- Among them are spectra of independent samples from 43 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tranexamic acid	21B05-F03-377271	2
	Tranexamic acid	2304017-01	4
	Tranexamic acid	2312001-01	1
AHD	Tranexamic acid	APX1712011MT	2
Audor Pharma	Tranexamic acid	1508016MT	1
Audor Pharma	Tranexamic acid	APX1508016MT	4
Audor Pharma	Tranexamic acid	APX1611013MT	6
Audor Pharma	Tranexamic acid	APX17112011MT	1
Audor Pharma	Tranexamic acid	APX1712011MT	8
Audor Pharma	Tranexamic acid	ApX1803027MT	1
Audor Pharma	Tranexamic acid	APX1803027MT	6
Audor Pharma	Tranexamic acid	X1611013M	2
Audor Pharma	Tranexamic acid	X1706014M	1
Audor Pharma	Tranexamic acid	X1712011M	1
Audor Pharma	Tranexamic acid	X1803027M	1
Caelo	Tranexamic acid	15J29-B04	1
Caelo	Tranexamic acid	16E31-B07-331591	1
Caelo	Tranexamic acid	18/25-B05-354991	1
Caelo	Tranexamic acid	18A17-B05-345037	1
Caelo	Tranexamic acid	2006030-02	1
Caelo	Tranexamic acid	APX1712011MT	1
Euro OTC	Tranexamic acid		1
Euro OTC	Tranexamic acid	2002005-01	1
Euro OTC	Tranexamic acid	2006030-01	11
Euro OTC	Tranexamic acid	2006030-02	1
Euro OTC	Tranexamic acid	2203031-01	1
Euro OTC	Tranexamic acid	TXAA200005	1
Fagron	Tranexamic acid	1197-18-8	1
Fagron	Tranexamic acid	12D11-N02	1
Fagron	Tranexamic acid	13D08-N24	1
Fagron	Tranexamic acid	13D08-N240002/40	1
Fagron	Tranexamic acid	13Do8-N24	1
Fagron	Tranexamic acid	13G24-N21	1
Fagron	Tranexamic acid	13K08-B04-287966	1
Fagron	Tranexamic acid	15J29-B04	1
Fagron	Tranexamic acid	15J29-B04-312372	1
Fagron	Tranexamic acid	16B03-B02-319617	2
Fagron	Tranexamic acid	16J29-B04-312372	1
Fagron	Tranexamic acid	18A17-B05-345037	1
Fagron	Tranexamic acid	18A17-B05-345038	1
Fagron	Tranexamic acid	18F20-B01	1
Fagron	Tranexamic acid	18F20-B01-351691	3
Fagron	Tranexamic acid	18F20-B01-351693	1
Fagron	Tranexamic acid	18J25-B05	1
Fagron	Tranexamic acid	18J25-B05-354991	4
Fagron	Tranexamic acid	20H24-F02	1
Fagron	Tranexamic acid	20H24F02373687	1
Fagron	Tranexamic acid	20H24-F02-373687	2
Fagron	Tranexamic acid	21B05-F03-377271	2
Fagron	Tranexamic acid	5041804	1
Fagron	Tranexamic acid	F02-3736807	1
Fagron	Tranexamic acid	X1712011M	1
Fagron	Tranexamic acid	X19D25-B01-361249	1
Fagron	Tranexamic acid	X2012306M	1
Noweda	Tranexamic acid	18a17-b05-345037	1
Sanacorp	Tranexamic acid	16E31-B07-331591	1
Sanacorp	Tranexamic acid	2002005-02	1
Sanacorp	Tranexamic acid	2006030-01	1

- 235 965 spectra from 1515 *Apo-Ident* customers from a total of 49 210 batches from a further

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tranexamic acid* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tranexamic acid* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	240	0	201 844
Type C	0	102	0	235 965

The substance/substance group *Tranexamic acid* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.5000 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 94.1176 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21654	21654	0.00	119.50
21727	21727	0.00	112.39
23504	25099	4.08	111.52
24708	25099	4.34	117.14
25078	25078	0.00	109.47
25099	25099	0.00	114.59
25586	25078	9.32	119.17
26652	26652	0.00	118.93
27140	27140	0.00	121.90

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tretinoin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20474-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tretinoin; Tretinoinum

Special notes

When selecting the *Tretinoin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tretinoin	6	18	333

Second-stage model

For differentiation of the substance/substance group *Tretinoin* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tretinoin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Mepivacaine hydrochloride	69.10	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tretinoin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tretinoin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Tretinoin	15028403	21757	60	1507086
Caelo	Tretinoin	15028403	21757SI	60	1507086
Caelo	Tretinoin	15239503	21878	60	20150717
Caelo	Tretinoin	15239503	21878SI	60	20150717
Euro OTC	Tretinoin	1402007-02	21747	60	1507085
Euro OTC	Tretinoin	1402007-02	21747SI	60	1507085
Euro OTC	Tretinoin	1510007	21940	60	20151102*
Euro OTC	Tretinoin	1510007	21940SI	60	20151102*
Euro OTC	Tretinoin	1604059	22574	40	20160603*
Fagron	Tretinoin	15F01-B06-317884	22936	40	20150619
Fagron	Tretinoin	15F01-B06-317884	22936SI	40	20150619

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 600 spectra of 11 reference samples from the substance/substance group *Tretinoin*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 362 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1460 spectra of 37 reference samples from the substance/substance group *Tretinoin*.

- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Tretinoin	162915	22779	40
Caelo	Tretinoin	162171	22780	40
Caelo	Tretinoin	172731	23680	40
Caelo	Tretinoin	173057	23843	40
Caelo	Tretinoin	181673	24251	40
Caelo	Tretinoin	181674	24258	40
Euro OTC	Tretinoin	1612010	22911	40
Euro OTC	Tretinoin	1804005	24061	40
Euro OTC	Tretinoin	1901001	24456	40
Euro OTC	Tretinoin	1907014	24855	40
Euro OTC	Tretinoin	2004014	25283	40
Euro OTC	Tretinoin	2106017	25779	40
Euro OTC	Tretinoin	2205021	26228	40
Euro OTC	Tretinoin	2303017	26655	40
Euro OTC	Tretinoin	2311013	27198	40
Euro OTC	Tretinoin	2406007	27407	40
Fagron	Tretinoin	18J30-B02-358547	24824	40
Fagron	Tretinoin	22F28-B05-221065	26606	40
Caelo	Tretinoin	162915	22779SI	40
Caelo	Tretinoin	162171	22780SI	40
Caelo	Tretinoin	172731	23680SI	40
Caelo	Tretinoin	173057	23843SI	40
Caelo	Tretinoin	181673	24251SI	20
Caelo	Tretinoin	181674	24258SI	40
Euro OTC	Tretinoin	1604059	22574SI†	40
Euro OTC	Tretinoin	1612010	22911SI	40
Euro OTC	Tretinoin	1804005	24061SI	40
Euro OTC	Tretinoin	1901001	24456SI	40
Euro OTC	Tretinoin	1907014	24855SI	40

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Tretinoin	2004014	25283SI	40
Euro OTC	Tretinoin	2106017	25779SI	40
Euro OTC	Tretinoin	2205021	26228SI	40
Euro OTC	Tretinoin	2303017	26655SI	40
Euro OTC	Tretinoin	2311013	27198SI	40
Euro OTC	Tretinoin	2406007	27407SI	40
Fagron	Tretinoin	18J30-B02-358547	24824SI	40
Fagron	Tretinoin	22F28-B05-221065	26606SI	40

- 200 624 spectra from a total of 4026 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1649 spectra from 729 *Apo-Ident* customers from 340 batches from the substance/substance group *Tretinoin*.
- Among them are spectra of independent samples from 332 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Tretinoin	2004014-02	1
	Tretinoin	2100421009	1
	Tretinoin	21004211007	1
	Tretinoin	2106017-02	4
	Tretinoin	2106017-03	1
	Tretinoin	21G10-B08-213327	1
	Tretinoin	2205021-01	6
	Tretinoin	2205021-02	9
	Tretinoin	2205321-02	1
	Tretinoin	22120002	1
	Tretinoin	22F28-B05-221065	1
	Tretinoin	2303017	4
	Tretinoin	2303017-01	18
	Tretinoin	23A23-B12-225240	1
	Tretinoin	24000848003	1
AHC	Tretinoin	2205021-02	1
AHD	Tretinoin	16070002	1
AHD	Tretinoin	1901001-01	1
AHD	Tretinoin	1907014-02	1
AHD	Tretinoin	2311013-01	1
Alliance Healthcare	Tretinoin	20000490002	1
Alliance Healthcare	Tretinoin	2205021-01	1
Allianz Healthcare	Tretinoin	1907014-01	1
Anzag/Henry Lamotte	Tretinoin	15078303	1
Anzag	Tretinoin	14L24B01303157	1
Anzag	Tretinoin	15078305	1
Apo Ident/ Noweda	Tretinoin	1804005-01	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
apo-ident	Tretinoin	1804005-01	1
Apo-ident	Tretinoin	2004014-01	1
apomix	Tretinoin	8806694	1
BASF / Phönix	Tretinoin	1604059-02	1
BASF/Phönix	Tretinoin	1304028-02	2
BASF	Tretinoin	1402007-03	1
Bombastus	Tretinoin	1402007-03	1
Caelo	Tretinoin		1
Caelo	Tretinoin	10003050032	1
Caelo	Tretinoin	1109014-02	1
Caelo	Tretinoin	11225504	1
Caelo	Tretinoin	11225506	1
Caelo	Tretinoin	11225511	1
Caelo	Tretinoin	11284703	1
Caelo	Tretinoin	12023302	9
Caelo	Tretinoin	12023303	1
Caelo	Tretinoin	12023309	1
Caelo	Tretinoin	12102902	1
Caelo	Tretinoin	12102903	2
Caelo	Tretinoin	12102904	2
Caelo	Tretinoin	12320201	2
Caelo	Tretinoin	12320203	2
Caelo	Tretinoin	12320204	1
Caelo	Tretinoin	12320205	5
Caelo	Tretinoin	12320207	1
Caelo	Tretinoin	12320209	6
Caelo	Tretinoin	12320301	1
Caelo	Tretinoin	12320303	1
Caelo	Tretinoin	12367101	2
Caelo	Tretinoin	12367103	2
Caelo	Tretinoin	12367104	1
Caelo	Tretinoin	12959AX20	1
Caelo	Tretinoin	12D05-N08	1
Caelo	Tretinoin	12I06-N01	1
Caelo	Tretinoin	1304028-02	3
Caelo	Tretinoin	131950002	1
Caelo	Tretinoin	13195002	14
Caelo	Tretinoin	13195003	1
Caelo	Tretinoin	13195008	1
Caelo	Tretinoin	13278101	1
Caelo	Tretinoin	13278102	4
Caelo	Tretinoin	13278104	2
Caelo	Tretinoin	13278105	2
Caelo	Tretinoin	13308003	1
Caelo	Tretinoin	13308004	4
Caelo	Tretinoin	13B05-B02-287360	1
Caelo	Tretinoin	14040504	5
Caelo	Tretinoin	14040507	1
Caelo	Tretinoin	14093502	4
Caelo	Tretinoin	14093503	1
Caelo	Tretinoin	1411016-01	2
Caelo	Tretinoin	14252702	5
Caelo	Tretinoin	14252706	2
Caelo	Tretinoin	14252710	2
Caelo	Tretinoin	14252801	1
Caelo	Tretinoin	1452802	1
Caelo	Tretinoin	14L24-B01-303157	2
Caelo	Tretinoin	15078301	1
Caelo	Tretinoin	15078302	2
Caelo	Tretinoin	15078303	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tretinoin	15078305	2
Caelo	Tretinoin	15078307	3
Caelo	Tretinoin	15078308	1
Caelo	Tretinoin	151000701	1
Caelo	Tretinoin	1510007-02	2
Caelo	Tretinoin	1517E-02563	1
Caelo	Tretinoin	15239501	2
Caelo	Tretinoin	15239502	6
Caelo	Tretinoin	15239503	2
Caelo	Tretinoin	15437301	1
Caelo	Tretinoin	15437303	14
Caelo	Tretinoin	15F01-B06-308856	1
Caelo	Tretinoin	15H31-B01	1
Caelo	Tretinoin	160405901	1
Caelo	Tretinoin	1604059-02	1
Caelo	Tretinoin	16070001	1
Caelo	Tretinoin	16070002	2
Caelo	Tretinoin	16070003	1
Caelo	Tretinoin	1612010-01	4
Caelo	Tretinoin	1612010-02	2
Caelo	Tretinoin	16217107	1
Caelo	Tretinoin	16217108	3
Caelo	Tretinoin	16217112	2
Caelo	Tretinoin	16217120	1
Caelo	Tretinoin	16217122	3
Caelo	Tretinoin	16291502	6
Caelo	Tretinoin	16291503	8
Caelo	Tretinoin	16357602	1
Caelo	Tretinoin	16F14-B04	1
Caelo	Tretinoin	16F14-B04-324636	1
Caelo	Tretinoin	16F14-B04-326181	1
Caelo	Tretinoin	16K03-806328-388	1
Caelo	Tretinoin	17106101	4
Caelo	Tretinoin	17106102	15
Caelo	Tretinoin	171061025343	1
Caelo	Tretinoin	17106103	1
Caelo	Tretinoin	1723102	1
Caelo	Tretinoin	17273102	1
Caelo	Tretinoin	17273103	1
Caelo	Tretinoin	172773102	1
Caelo	Tretinoin	17305701	10
Caelo	Tretinoin	17305702	7
Caelo	Tretinoin	17305704	6
Caelo	Tretinoin	17305705	1
Caelo	Tretinoin	17305707	6
Caelo	Tretinoin	173057075597	1
Caelo	Tretinoin	17305708	1
Caelo	Tretinoin	17305709	2
Caelo	Tretinoin	17305710	2
Caelo	Tretinoin	17305711	1
Caelo	Tretinoin	17357001	11
Caelo	Tretinoin	17357002	7
Caelo	Tretinoin	17357004	1
Caelo	Tretinoin	17357005	2
Caelo	Tretinoin	17357007	7
Caelo	Tretinoin	17357008	4
Caelo	Tretinoin	17357009	5
Caelo	Tretinoin	1735707	1
Caelo	Tretinoin	17K01-B05-0005	1
Caelo	Tretinoin	17K01-B05-345784	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tretinoin	1804005-01	9
Caelo	Tretinoin	18167301	3
Caelo	Tretinoin	18167301P-190314-2	1
Caelo	Tretinoin	18167302	9
Caelo	Tretinoin	18167307	5
Caelo	Tretinoin	18167309	22
Caelo	Tretinoin	18167401	6
Caelo	Tretinoin	18167402	4
Caelo	Tretinoin	18167403	2
Caelo	Tretinoin	18167405	2
Caelo	Tretinoin	18167407	1
Caelo	Tretinoin	18167408	1
Caelo	Tretinoin	18167409	3
Caelo	Tretinoin	18167410	3
Caelo	Tretinoin	1901001-01	4
Caelo	Tretinoin	1903084002	1
Caelo	Tretinoin	190500003	1
Caelo	Tretinoin	19050001	13
Caelo	Tretinoin	19050003	18
Caelo	Tretinoin	1907014-01	1
Caelo	Tretinoin	1907014-02	1
Caelo	Tretinoin	191001-01	1
Caelo	Tretinoin	19185802	5
Caelo	Tretinoin	19185803	3
Caelo	Tretinoin	19185805	12
Caelo	Tretinoin	19185808	1
Caelo	Tretinoin	192571001	1
Caelo	Tretinoin	192571002	1
Caelo	Tretinoin	192571003	1
Caelo	Tretinoin	192571005	1
Caelo	Tretinoin	19257102	6
Caelo	Tretinoin	19257103	6
Caelo	Tretinoin	193084002	12
Caelo	Tretinoin	193084003	11
Caelo	Tretinoin	20000490001	5
Caelo	Tretinoin	20000490002	8
Caelo	Tretinoin	20000490005	5
Caelo	Tretinoin	20001881004	7
Caelo	Tretinoin	20004135001	7
Caelo	Tretinoin	20004135002	1
Caelo	Tretinoin	2004014-0	1
Caelo	Tretinoin	2004014-01	2
Caelo	Tretinoin	2004014-02	1
Caelo	Tretinoin	20120601	1
Caelo	Tretinoin	20A28-F01-368810	1
Caelo	Tretinoin	21000305002	8
Caelo	Tretinoin	21000305003	9
Caelo	Tretinoin	21000703001	7
Caelo	Tretinoin	21000703002	4
Caelo	Tretinoin	21000703004	3
Caelo	Tretinoin	21004211002	5
Caelo	Tretinoin	21004211003	12
Caelo	Tretinoin	21004211005	1
Caelo	Tretinoin	21004211007	3
Caelo	Tretinoin	2100421107	1
Caelo	Tretinoin	2205021-01	1
Caelo	Tretinoin	3041302	1
Caelo	Tretinoin	5012I-02563	1
Caelo	Tretinoin	711212563	1
Caeol/Noweda	Tretinoin	15437303	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz /Gehe	Tretinoin	193084003	1
Caesar & Loretz GmbH...	Tretinoin	21004211002	1
Caesar & Loretz GmbH...	Tretinoin	12023302	1
Caesar & Loretz GmbH...	Tretinoin	21004211005	1
Caesar & Loretz GmbH...	Tretinoin	193084003	1
Caesar & Loretz GmbH...	Tretinoin	19050001	1
Caesar & Loretz GmbH...	Tretinoin	20000490005	1
Caesar & Loretz GmbH/AHD	Tretinoin	19257103	1
Caesar & Loretz GmbH/AHD	Tretinoin	20000490002	1
Caesar & Loretz GmbH/AHD	Tretinoin	21000305002	1
Caesar & Loretz GmbH...	Tretinoin	19185802	1
Caesar & Loretz GmbH...	Tretinoin	20000490001	1
Caesar & Loretz GmbH...	Tretinoin	21000305002	2
Caesar & Loretz GmbH...	Tretinoin	193084002	1
Caesar & Loretz GmbH...	Tretinoin	19257103	2
Caesar & Loretz GmbH...	Tretinoin	193084002	1
Caesar & Loretz GmbH/gehe	Tretinoin	19257102	1
Caesar & Loretz GmbH/Gehe	Tretinoin	21000305003	1
Caesar & Loretz GmbH...	Tretinoin	21000703002	1
Caesar & Loretz GmbH...	Tretinoin	19185803	1
Caesar & Loretz GmbH...	Tretinoin	193084002	1
Caesar & Loretz GmbH...	Tretinoin	21000302002	1
Caesar & Loretz GmbH...	Tretinoin	21000305002	2
Caesar & Loretz GmbH/Sana	Tretinoin	193084003	1
Caesar & Loretz GmbH...	Tretinoin	21004211006	1
Caesar & Loretz GmbH...	Tretinoin	22002262001	1
Caesar & Loretz GmbH...	Tretinoin	193084002	1
Caesar & Loretz GmbH	Tretinoin	11225515	1
Caesar & Loretz GmbH	Tretinoin	12320211	1
Caesar & Loretz GmbH	Tretinoin	18167302	1
Caesar & Loretz GmbH	Tretinoin	18167309	1
Caesar & Loretz GmbH	Tretinoin	18167401	1
Caesar & Loretz GmbH	Tretinoin	18167408	1
Caesar & Loretz GmbH	Tretinoin	18167410	1
Caesar & Loretz GmbH	Tretinoin	19050001	2
Caesar & Loretz GmbH	Tretinoin	19050003	4
Caesar & Loretz GmbH	Tretinoin	19185801	1
Caesar & Loretz GmbH	Tretinoin	19185802	1
Caesar & Loretz GmbH	Tretinoin	19185803	2
Caesar & Loretz GmbH	Tretinoin	19185805	1
Caesar & Loretz GmbH	Tretinoin	192571001	1
Caesar & Loretz GmbH	Tretinoin	19257102	1
Caesar & Loretz GmbH	Tretinoin	19257103	4
Caesar & Loretz GmbH	Tretinoin	193084002	1
Caesar & Loretz GmbH	Tretinoin	193084003	6
Caesar & Loretz GmbH	Tretinoin	20000490001	2
Caesar & Loretz GmbH	Tretinoin	20000490002	4
Caesar & Loretz GmbH	Tretinoin	20000490005	1
Caesar & Loretz GmbH	Tretinoin	20001881004	2
Caesar & Loretz GmbH	Tretinoin	20001881005	1
Caesar & Loretz GmbH	Tretinoin	21000305001	1
Caesar & Loretz GmbH	Tretinoin	21000305002	1
Caesar & Loretz GmbH	Tretinoin	21000305003	9
Caesar & Loretz GmbH	Tretinoin	21000703001	5
Caesar & Loretz GmbH	Tretinoin	21000703004	1
Caesar & Loretz GmbH	Tretinoin	21004211002	2
Caesar & Loretz GmbH	Tretinoin	21004211003	2
Caesar & Loretz GmbH	Tretinoin	21004211005	3
Caesar & Loretz GmbH	Tretinoin	21004211007	1
Caesar & Loretz GmbH	Tretinoin	21004211009	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Cealo/Phoenix	Tretinoin	19050003	1
cealo	Tretinoin	13195002	1
Ceasar & Lorenz	Tretinoin	19185805	2
Celo/Kehr	Tretinoin	16217122	1
Celo	Tretinoin	15437303	1
Eu Rho	Tretinoin	1612010-02	1
Eur Rho	Tretinoin	200401402	1
EuRho / AHD	Tretinoin	2106017-02	1
EuRho / Phoenix	Tretinoin	2205021-01	1
EuRho- Phoenix	Tretinoin	2106017-01	1
EURho/ Noweda	Tretinoin	1901001-01	1
EuRho/ Fiebig	Tretinoin	2004014-01	1
EuRho/ NOWEDA	Tretinoin	1804005-01	2
EuRho/ Noweda	Tretinoin	1907014-02	1
EuRho/ Sanacorp	Tretinoin	2205021-02	3
Eurho/Noweda	Tretinoin	2004014-02	1
EURho/Phoenix	Tretinoin	1907014-01	1
Eurho/Phönix	Tretinoin	2205021	1
EuRho/Sanacorp	Tretinoin	130402802	1
EuRho/Sanacorp	Tretinoin	210601703	1
EuRho/Spangro	Tretinoin	1901001-01	1
EuRho	Tretinoin	151007-01	1
EuRho	Tretinoin	1804005-01	1
EuRho	Tretinoin	19042068	1
EuRho	Tretinoin	1907014-01	1
EuRho	Tretinoin	190701402	1
EuRho	Tretinoin	1907014-02	1
EuRho	Tretinoin	2004014-02	4
EuRho	Tretinoin	2205021-01	1
Eurimpharm	Tretinoin	1411016-01	1
Euro OCT Pharma/Fiebig	Tretinoin	1604059-01	2
Euro OT/ Gehe	Tretinoin	1901001-01	2
Euro OTC	Tretinoin	1008021-02	1
Euro OTC	Tretinoin	10429AX21	1
Euro OTC	Tretinoin	1109014-02	2
Euro OTC	Tretinoin	12059AX20	2
Euro OTC	Tretinoin	12959AX20	3
Euro OTC	Tretinoin	130102802	1
Euro OTC	Tretinoin	1304028-01	7
Euro OTC	Tretinoin	130402802	1
Euro OTC	Tretinoin	1304028-02	4
Euro OTC	Tretinoin	13041028-01	1
Euro OTC	Tretinoin	140007-02	1
Euro OTC	Tretinoin	14020007-01	1
Euro OTC	Tretinoin	1402007	1
Euro OTC	Tretinoin	140200701	1
Euro OTC	Tretinoin	1402007-01	5
Euro OTC	Tretinoin	1402007-02	9
Euro OTC	Tretinoin	140200703	1
Euro OTC	Tretinoin	1402007-03	3
Euro OTC	Tretinoin	14101602	1
Euro OTC	Tretinoin	1411016-01	12
Euro OTC	Tretinoin	141101602	1
Euro OTC	Tretinoin	1411016-02	12
Euro OTC	Tretinoin	141107602	1
Euro OTC	Tretinoin	151000	1
Euro OTC	Tretinoin	1510007-01	13
Euro OTC	Tretinoin	151000702	1
Euro OTC	Tretinoin	1510007-02	17
Euro OTC	Tretinoin	16004059-02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Tretinoin	160405901	1
Euro OTC	Tretinoin	1604059-01	23
Euro OTC	Tretinoin	160405902	2
Euro OTC	Tretinoin	1604059-02	21
Euro OTC	Tretinoin	16052905	1
Euro OTC	Tretinoin	161201001	2
Euro OTC	Tretinoin	1612010-01	30
Euro OTC	Tretinoin	1612010-02	15
Euro OTC	Tretinoin	161210-01	1
Euro OTC	Tretinoin	162010-02	1
Euro OTC	Tretinoin	16217108	1
Euro OTC	Tretinoin	165070002	1
Euro OTC	Tretinoin	17273103	1
Euro OTC	Tretinoin	17357001	2
Euro OTC	Tretinoin	17Ko1-Bo5-345784	1
Euro OTC	Tretinoin	180400501	4
Euro OTC	Tretinoin	1804005-01	49
Euro OTC	Tretinoin	1804008-01	1
Euro OTC	Tretinoin	18062082	2
Euro OTC	Tretinoin	18167302	1
Euro OTC	Tretinoin	18167405	1
Euro OTC	Tretinoin	184005-01	1
Euro OTC	Tretinoin	18432003	3
Euro OTC	Tretinoin	18J30-B02-359836	1
Euro OTC	Tretinoin	190100-01	1
Euro OTC	Tretinoin	190100101	2
Euro OTC	Tretinoin	1901001-01	44
Euro OTC	Tretinoin	190100102	1
Euro OTC	Tretinoin	1901001-02	20
Euro OTC	Tretinoin	19042068	3
Euro OTC	Tretinoin	19042092	3
Euro OTC	Tretinoin	1907014	1
Euro OTC	Tretinoin	190701401	4
Euro OTC	Tretinoin	1907014-01	22
Euro OTC	Tretinoin	190701402	1
Euro OTC	Tretinoin	1907014-02	42
Euro OTC	Tretinoin	190714-02	2
Euro OTC	Tretinoin	2001014-01	1
Euro OTC	Tretinoin	2001014-02	2
Euro OTC	Tretinoin	2004014	2
Euro OTC	Tretinoin	2004014-01	45
Euro OTC	Tretinoin	2004014-02	41
Euro OTC	Tretinoin	20332110	1
Euro OTC	Tretinoin	2105017-01	1
Euro OTC	Tretinoin	2106017	1
Euro OTC	Tretinoin	2106017_03	1
Euro OTC	Tretinoin	210601701	2
Euro OTC	Tretinoin	2106017-01	15
Euro OTC	Tretinoin	2106017-02	24
Euro OTC	Tretinoin	2106017-03	11
Euro OTC	Tretinoin	2205021-01	11
Euro OTC	Tretinoin	230301701	1
Euro OTC	Tretinoin	2303017-01	2
Euro OTC	Tretinoin	2994014-02	1
Euro OTC	Tretinoin	30042014A	1
Euro OTC	Tretinoin	5219Q-02563	1
Euro OTC	Tretinoin	67(1804005-01)	1
Euro OTC	Tretinoin	819081-16	1
Euro OTC	Tretinoin	99999999	1
Euro/Gehe	Tretinoin	1604059-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro/Noweda	Tretinoin	1612010-01	1
Euro/Phoenix	Tretinoin	1901001-01	2
Euro/Phoenix	Tretinoin	1907014-01	1
Euro/Phönix	Tretinoin	18J30B02359836	1
Euro/Phönix	Tretinoin	1907014-01	1
Euro/Sanacorp	Tretinoin	1604059-02	1
Euro	Tretinoin	14111016-01	1
Euroo/Phönix	Tretinoin	210601703	1
EuroPharm/ Sanacorp	Tretinoin	1804005-01	1
Fagron	Tretinoin	11K29-N01	1
Fagron	Tretinoin	12I06-N01	2
Fagron	Tretinoin	12106-N01	1
Fagron	Tretinoin	13B05-B02-287360	4
Fagron	Tretinoin	13B05-B02-287361	2
Fagron	Tretinoin	13C11-N06	2
Fagron	Tretinoin	13D30N14	1
Fagron	Tretinoin	13D30-N14	2
Fagron	Tretinoin	13D30-N14-3365319091	1
Fagron	Tretinoin	14009-804	1
Fagron	Tretinoin	14040504	1
Fagron	Tretinoin	14093505	1
Fagron	Tretinoin	1410001594	1
Fagron	Tretinoin	1411016-01	1
Fagron	Tretinoin	1440104	1
Fagron	Tretinoin	14D09-B04	1
Fagron	Tretinoin	14D09-B04-293224	1
Fagron	Tretinoin	14D09-B04-293225	1
Fagron	Tretinoin	14D09-B04-293594	1
Fagron	Tretinoin	14D09-B04-295551	1
Fagron	Tretinoin	14L24-B01	1
Fagron	Tretinoin	14L24-B01-303152	1
Fagron	Tretinoin	14L24-B01-303157	4
Fagron	Tretinoin	1510007-01	1
Fagron	Tretinoin	1510007-02	1
Fagron	Tretinoin	15F01-B06-308722	7
Fagron	Tretinoin	15F01-B06-308856	4
Fagron	Tretinoin	15F01-B06-313216	2
Fagron	Tretinoin	15F01-B06-315491	1
Fagron	Tretinoin	15F01-B06-317884	1
Fagron	Tretinoin	1604059-01	1
Fagron	Tretinoin	16052905	4
Fagron	Tretinoin	16F14-B04	3
Fagron	Tretinoin	16F14-B04-324636	2
Fagron	Tretinoin	16f14-b04-325560	1
Fagron	Tretinoin	16F14B04325560	1
Fagron	Tretinoin	16F14-B04-325560	2
Fagron	Tretinoin	16F-14-B04-325560	1
Fagron	Tretinoin	16F14-B04-325567	1
Fagron	Tretinoin	16F14-B04-326181	2
Fagron	Tretinoin	16F14BO4325560	1
Fagron	Tretinoin	16K03-B06	3
Fagron	Tretinoin	16K03-B06-328388	5
Fagron	Tretinoin	170706TTRER-20151004	1
Fagron	Tretinoin	17273102	1
Fagron	Tretinoin	17357007	1
Fagron	Tretinoin	17K01-B05	2
Fagron	Tretinoin	17K01-B05-341936	8
Fagron	Tretinoin	17K01-B05-341941	2
Fagron	Tretinoin	17K01-B05-345784	4
Fagron	Tretinoin	17K01-B05-347435	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Tretinoin	17K01-B05-347436	1
Fagron	Tretinoin	17K01B05349946	1
Fagron	Tretinoin	17K01-B05-349946	4
Fagron	Tretinoin	18167404	1
Fagron	Tretinoin	18A10-B03-344364	1
Fagron	Tretinoin	18J30-B02	2
Fagron	Tretinoin	18J30-B02_359836	1
Fagron	Tretinoin	18j30B02358540	1
Fagron	Tretinoin	18J30-B02-358540	4
Fagron	Tretinoin	18J30-B02-358546	1
Fagron	Tretinoin	18J30-B02-358547	1
Fagron	Tretinoin	18J30-B02-359836	1
Fagron	Tretinoin	18J30-B02-362110	5
Fagron	Tretinoin	18J30-B02-362120	1
Fagron	Tretinoin	19K07-06-366648	1
Fagron	Tretinoin	19K07-F06	4
Fagron	Tretinoin	19K07-F06-366648	12
Fagron	Tretinoin	20000490002	2
Fagron	Tretinoin	20110004	1
Fagron	Tretinoin	20120601	1
Fagron	Tretinoin	20A28-F01-368810	2
Fagron	Tretinoin	20A28-F01-368813	1
Fagron	Tretinoin	21E17-F03-378623	2
Fagron	Tretinoin	21G10-B08	1
Fagron	Tretinoin	21G10-B08-213327	2
Fagron	Tretinoin	22080001	1
Fagron	Tretinoin	231115T	1
Fagron	Tretinoin	23A23-B12-225240	1
Fagron	Tretinoin	6366648	1
Fagron	Tretinoin	F01-3688100	2
Fagron	Tretinoin	TRER-20180703	2
Fargon	Tretinoin	16K03-B06-328388	1
Fargron/ Sanacorp	Tretinoin	17k01-b05-341936	1
Fargron	Tretinoin	1402007-01	1
Fargron	Tretinoin	14D09-B04-293225	1
FEJ	Tretinoin	15F01-B06-308856	1
Fiebig	Tretinoin	1612010-01	1
Gatt-Koller	Tretinoin	1702180	1
Gatt-Koller	Tretinoin	1804193	1
Gatt-Koller	Tretinoin	606210909	1
Gehe am 11.10.2017	Tretinoin	17106102	1
Gehe amax	Tretinoin	1604059-02	1
Gehe	Tretinoin	15078307	1
Gehe	Tretinoin	1510007-01	1
Gehe	Tretinoin	15437303	1
Gehe	Tretinoin	1604059-02	1
Gehe	Tretinoin	1612010-01	1
Gehe	Tretinoin	1901001-01	1
Gehe	Tretinoin	1901001-02	1
Gehe	Tretinoin	19050001	1
GEHE	Tretinoin	19050001	1
Gehe	Tretinoin	1907014-01	2
Gehe	Tretinoin	1907014-02	1
Gehe	Tretinoin	2106017-01	1
Gehe	Tretinoin	2205021-02	1
GEHE	Tretinoin	2205021-02	1
Gehe-Eurho 22.11.2017	Tretinoin	2171127Ma7	1
Geibo	Tretinoin	17K01-B05-341936	1
JENNE	Tretinoin	17K01-B05-341941	1
Jenne	Tretinoin	1901001-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Kehr	Tretinoin	1604059-01	1
Krieger am 17.08.2018	Tretinoin	17K01-B05-345784	1
Krieger	Tretinoin	1612010-02	2
Krieger	Tretinoin	2205021-02	1
L10	Tretinoin	1612010-01	2
Nachprüfung	Tretinoin		1
Nachprüfung	Tretinoin	2605001-01	1
Noweda/EuRho 06.05.2...	Tretinoin	2004014-01	1
Noweda/EuRho	Tretinoin	2106017-02	1
Noweda	Tretinoin	12023302	2
Noweda	Tretinoin	13D30-N14	1
Noweda	Tretinoin	15078307	1
Noweda	Tretinoin	15F01-B06-315491	1
Noweda	Tretinoin	17305701	1
Noweda	Tretinoin	1804005-01	3
Noweda	Tretinoin	18167402	1
Noweda	Tretinoin	19257103	1
Noweda	Tretinoin	200401402	1
Noweda	Tretinoin	2004014-02	1
Noweda	Tretinoin	2205021-01	2
Noweda	Tretinoin	2205021-02	1
Phoenix	Tretinoin	12367103	1
Phoenix	Tretinoin	15F01-B06-317884	1
Phoenix	Tretinoin	190701402	1
Phoenix	Tretinoin	19K07-F06-366648	1
Phoenix	Tretinoin	200401401	3
Phoenix	Tretinoin	2004014-01	3
Phoenix	Tretinoin	2106017-03	1
Phoenix	Tretinoin	2205021-02	1
Phönix WE:04.01.18 ...	Tretinoin	17273102	1
Phönix	Tretinoin	1109014-02	1
Phönix	Tretinoin	1402007-02	1
Phönix	Tretinoin	14D09-B04	2
Phönix	Tretinoin	14D09-B04-293224	1
phönix	Tretinoin	1612010-01	1
phönix	Tretinoin	17273102	1
Phönix	Tretinoin	17k01-b05-349946	1
Phönix	Tretinoin	18167302	1
Phönix	Tretinoin	1901001-01	1
Phönix	Tretinoin	200831409	1
Phönix	Tretinoin	200931709	1
Phönix	Tretinoin	2205021-01	1
Phönix	Tretinoin	3144	1
Sana	Tretinoin	21G10-B08-213327	1
Sanacorp/EuRho	Tretinoin	1604059-02	1
Sanacorp	Tretinoin	12/06-N01	1
Sanacorp	Tretinoin	12320302	1
Sanacorp	Tretinoin	13308004	1
Sanacorp	Tretinoin	1411016-01	1
Sanacorp	Tretinoin	1411016-02	1
Sanacorp	Tretinoin	14L24-B01	1
Sanacorp	Tretinoin	16217122	1
Sanacorp	Tretinoin	17357001	1
Sanacorp	Tretinoin	1804005-01	1
Sanacorp	Tretinoin	18167309	1
Sanacorp	Tretinoin	1907014-02	1
Sanacorp	Tretinoin	19185805	1
Sanacorp	Tretinoin	193084003	1
Sanacorp	Tretinoin	21000305001	1
Sanacorp	Tretinoin	2205021-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Tretinoin	2303017-01	1
Sanacorp	Tretinoin	2311013-01	1
Siegfried Chemikalie…	Tretinoin	1804005	1
Siegfried Pharamchikalien	Tretinoin	2004014-01	1
Siegfried Pharm. Che…	Tretinoin	17K01-B05-345784	1
Siegfried Pharma / Gehe	Tretinoin	1907014-01	1
Siegfried Pharma / Gehe	Tretinoin	1907014-02	1
siegfried pharma che…	Tretinoin	2106017-01	1
Siegfried PharmaChem…	Tretinoin	1907014-02	1
Siegfried Pharmachem…	Tretinoin	2004014-01	1
Siegfried Pharmachem…	Tretinoin	19042092	1
Siegfried Pharmachem…	Tretinoin	2004014-01	1
Siegfried Pharmachem…	Tretinoin	2004014-02	1
Siegfried PharmaChem…	Tretinoin	18432003	1
Siegfried PharmaChem…	Tretinoin	19042092	1
Synthetisch/GEIBO	Tretinoin	2106017-03	1
synthetisch	Tretinoin	2106017-02	1
WE:Phönix 20.08.201…	Tretinoin	1510007-02	1
WE:Phönix 02.11..201…	Tretinoin	1604059-01	1

- 234 418 spectra from 1515 *Apo-Ident* customers from a total of 48 925 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tretinoin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tretinoin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	600	0	152 362
Type B	0	1460	0	200 624
Type C	0	1569	80	234 418

The substance/substance group *Tretinoin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.5890 %)
Type C	100.0000 % (> 99.9007 %)	95.1486 % (> 94.9666 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21747	21747	0.00	128.52
21757	21757	0.00	105.87
21878	21747	21.99	120.80
21940	21940	0.00	119.65
22574	22574	0.00	109.65
22936	21940	7.04	113.46

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Triamcinolone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20564-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Triamcinolone; Triamcinolonum

Special notes

When selecting the *Triamcinolone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Triamcinolone	9	3	58

Second-stage model

For differentiation of the substance/substance group *Triamcinolone* the following second-stage model is used:

- Submodel 03

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Triamcinolone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Riboflavin sodium phosphate hydrate	66.53	–
⋮	⋮	⋮
Cyanocobalamin	>50	36.47
Polymyxin B sulfate	67.00	38.25
Bacitracin	>50	42.86
Amphotericin B	>50	50.61
Colistin sulfate	>50	56.25
Riboflavin	>50	56.97
Methylcobalamin	>50	62.62
Calcium pantothenate	>50	67.49
Nystatin	>50	85.37
Estradiol hemihydrate	>50	90.28
Estriol	>50	95.20
Hyoscine hydrobromide	>50	103.27
Tosylchloramide sodium	>50	114.53
Gelatine, white	>50	115.38
alpha-tocopheryl acetate dry concentrate	>50	147.74
Calcium glycerophosphate	>50	150.96
Selenium yeast	>50	187.33
SyrSpend® SF pH4 neo (Maize starch)	>50	187.44
SyrSpend® SF Alka	>50	202.10
Oxalic acid	>50	223.18
Rice starch	>50	248.31
Carmellose sodium	>50	254.47
Corn starch	>50	339.13
SyrSpend® SF pH4	>50	348.51
Acacia, dried dispersion	>50	392.17
Wheat starch	>50	409.92
Maltodextrin	>50	462.17
Potato starch	>50	464.46
Fructose	>50	469.05

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Triamcinolone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Triamcinolone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Triamcinolone	15106905	22273	45	20150527
Caelo	Triamcinolone	15106905	22605	40	20150527
Caelo	Triamcinolone	20001706	25555	40	20200902*
Caelo	Triamcinolone	20001706	25555SI	35	20200902*
Fagron	Triamcinolone	12A03-N09	20730	40	20120117
Fagron	Triamcinolone	12K07-N13	20936	80	AR-15-FG-003373-01
Fagron	Triamcinolone	14B13-B30-316101	22840	40	20140311
Fagron	Triamcinolone	18A19-B05-351174	24182	40	1811263
Fagron	Triamcinolone	18A19-B05-351174	24182SI	32	1811263
Fagron	Triamcinolone	18E09-B04-353921	24446	40	1907730
Fagron	Triamcinolone	18J01-B05-364078	24944	40	2004435
Fagron	Triamcinolone	22A17-B05-216480	26140	40	20220421

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 512 spectra of 12 reference samples from the substance/substance group *Triamcinolone*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.
- 152 450 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 400 spectra of 10 reference samples from the substance/substance group *Triamcinolone*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Triamcinolone	15106911	23508	40
Fagron	Triamcinolone	17G03-B04-343670	24097	40
Fagron	Triamcinolone	21H13-B19-215838	25938	40
Fagron	Triamcinolone	17G03-B04-343670	24097SI	40
Fagron	Triamcinolone	17G03-B04-343670	24107	40
Fagron	Triamcinolone	17G03-B04-343670	24107SI	40
Fagron	Triamcinolone	18E09-B04-353921	24446SI†	40
Fagron	Triamcinolone	18J01-B05-364078	24944SI†	40
Fagron	Triamcinolone	21H13-B19-215838	25938SI	40
Fagron	Triamcinolone	22A17-B05-216480	26140SI†	40

- 201 684 spectra from a total of 4039 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 95 spectra from 58 *Apo-Ident* customers from 62 batches from the substance/substance group *Triamcinolone*.

- Among them are spectra of independent samples from 58 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Triamcinolone	22A17-B05-222384	1
	Triamcinolone	22J05B05227276	1
	Triamcinolone	22J05-B05-227276	2
Caelo	Triamcinolone	12295207	3
Caelo	Triamcinolone	12295210	1
Caelo	Triamcinolone	13J07-N08	2
Caelo	Triamcinolone	14B13-B30-293474	1
Caelo	Triamcinolone	14B13-B30312868	1
Caelo	Triamcinolone	15106902	1
Caelo	Triamcinolone	15106912	1
Caelo	Triamcinolone	15106960	1
Caelo	Triamcinolone	180921002	3
Caelo	Triamcinolone	18092104	3
Caesar & Loretz GmbH...	Triamcinolone	21001467001	1
Caesar & Loretz GmbH	Triamcinolone	21001467001	1
Fagron	Triamcinolone	11D28-N04	1
Fagron	Triamcinolone	11G26-N04	1
Fagron	Triamcinolone	12A03-N09	1
Fagron	Triamcinolone	12D02-N14	1
Fagron	Triamcinolone	12Do2-N14	1
Fagron	Triamcinolone	12F01-N19	3
Fagron	Triamcinolone	13C26-N04	1
Fagron	Triamcinolone	13D30-N15	2
Fagron	Triamcinolone	13J07-N08	1
Fagron	Triamcinolone	14A14-B01	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triamcinolone	14B13-B30	1
Fagron	Triamcinolone	14B13-B30-293473	1
Fagron	Triamcinolone	14B13-B30-312868	1
Fagron	Triamcinolone	14B13-B30-316102	1
Fagron	Triamcinolone	15B13-B30-312868	1
Fagron	Triamcinolone	16A13-B06	2
Fagron	Triamcinolone	18A19-B05-352984	3
Fagron	Triamcinolone	18E09-B04-355656	1
Fagron	Triamcinolone	18J01-B05	2
Fagron	Triamcinolone	18J01-B05-364078	2
Fagron	Triamcinolone	18J01B05364080	1
Fagron	Triamcinolone	18J01-B05-364080	1
Fagron	Triamcinolone	20k25-f03	1
Fagron	Triamcinolone	20K25-F03	2
Fagron	Triamcinolone	20K25-F03-376111	2
Fagron	Triamcinolone	20K25-F03-376112	4
Fagron	Triamcinolone	20K25-F03-377107	1
Fagron	Triamcinolone	21I03-B01-216482	1
Fagron	Triamcinolone	21l03-B01_216482	1
Fagron	Triamcinolone	21l03-B01-216482	1
Fagron	Triamcinolone	22A17-B05	1
Fagron	Triamcinolone	22A17-B05-216480	3
Fagron	Triamcinolone	F03-3761102	1
Fagron	Triamcinolone	NT1484M	1
Fagron	Triamcinolone	NTL171102	1
Fagron	Triamcinolone	NTL200702	2
Fargon/Gehe	Triamcinolone	B04-3539201	1
Fargon/Gehe	Triamcinolone	B05-3640708	1
Fargon	Triamcinolone	18J01-B05-364078	1
Gehe	Triamcinolone	16F07-B01-331398	1
Gehe	Triamcinolone	NTL180603	1
L12	Triamcinolone	17359001	1
Noweda 24.08.2015	Triamcinolone	14B13-B30-293474	1
Noweda	Triamcinolone	21/03-B01-216482	2
Noweda	Triamcinolone	22A17-B05-222384	1
Noweda	Triamcinolone	22J05-B05-227276	1
Phönix	Triamcinolone	18A19B05-352890	1
Phönix	Triamcinolone	NS0608M	1
Sanacorp	Triamcinolone	100/AKD6	1
Sanacorp	Triamcinolone	15106907	1
Sanacorp	Triamcinolone	15106916	1
Sanacorp	Triamcinolone	23F26-B02-229454	2
Tianjin Tianyao Phar...	Triamcinolone	18J01-B05-364080	1
Tianjin Tianyao Phar...	Triamcinolone	21I03-B01-216482	1

- 235 972 spectra from 1515 *Apo-Ident* customers from a total of 49 197 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Triamcinolone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Triamcinolone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following

table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	512	0	152 450
Type B	0	384	16	201 684
Type C	0	88	7	235 972

The substance/substance group *Triamcinolone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8281 %)
Type B	100.0000 % (> 99.9912 %)	96.0000 % (> 95.2500 %)
Type C	100.0000 % (> 99.9007 %)	92.6316 % (> 89.4737 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20730	20936	50.54	150.17
20936	20936	0.00	183.24
22273	25555	12.72	184.88
22605	25555	9.37	179.99
22840	25555	12.40	178.74
24182	24182	0.00	112.46
24446	24446	0.00	124.59
24944	24944	0.00	103.03
25555	25555	0.00	181.88
26140	24182	42.93	109.47

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Triamcinolone acetonide**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20765-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Triamcinolone acetonide; Triamcinoloni acetonidum

Special notes

When selecting the *Triamcinolone acetonide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Triamcinolone acetonide	12	24	810

Second-stage model

For differentiation of the substance/substance group *Triamcinolone acetonide* the following second-stage model is used:

- Submodel 02

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Triamcinolone acetonide* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Prednisolon dihydrogen phosphate di…	63.83	–
⋮	⋮	⋮
Fluocinolone acetonide	73.86	34.92
Prednisolone	>50	61.12
Betamethasone	>50	63.08
Methylprednisolone	>50	77.88
Tyrothricin	>50	90.87
Dexamethasone	>50	96.52
Gramicidin	>50	136.76

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Triamcinolone acetonide* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Triamcinolone acetonide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Triamcinolone acetonide	13256607	21061	100	AR-15-FG-003755-01
Caelo	Triamcinolone acetonide	13379921	21587	60	1503634
Caelo	Triamcinolone acetonide	20002630	25560	40	20200902*
Caelo	Triamcinolone acetonide	20002630	25560SI	31	20200902*
Euro OTC	Triamcinolone acetonide	1303001-02	20910	40	20130815
Euro OTC	Triamcinolone acetonide	1211013-02	21072	30	20130417
Euro OTC	Triamcinolone acetonide	1508008	21883	60	20150902*
Euro OTC	Triamcinolone acetonide	1601021	22313	45	20160119*
Euro OTC	Triamcinolone acetonide	1605010	22572	40	20160531*
Euro OTC	Triamcinolone acetonide	1605010	22572SI	25	20160531*
Euro OTC	Triamcinolone acetonide	1608005	22752	40	20160906*
Euro OTC	Triamcinolone acetonide	1608005	22752SI	22	20160906*
Euro OTC	Triamcinolone acetonide	2006002	25339	40	2011401

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Triamcinolone acetonide	2006002	25339SI	29	2011401
Fagron	Triamcinolone acetonide	12E15-N03	20765	60	1412051
Fagron	Triamcinolone acetonide	15C19-B06-308572	21962	60	20150402

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 722 spectra of 16 reference samples from the substance/substance group *Triamcinolone acetonide*. These samples are listed above in the *calibration samples* section. The reference samples come from 12 different batches.

- 152 240 spectra from a total of 2830 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1679 spectra of 50 reference samples from the substance/substance group *Triamcinolone acetonide*.

- Among them are spectra of independent samples from 24 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Triamcinolone acetonide	12301505	20769	60
Caelo	Triamcinolone acetonide	160945	22473	60
Caelo	Triamcinolone acetonide	171206	23330	40
Caelo	Triamcinolone acetonide	181002	24016	40
Caelo	Triamcinolone acetonide	190619	24509	40
Caelo	Triamcinolone acetonide	23002617	26965	40
Euro OTC	Triamcinolone acetonide	1612014	22978	40
Euro OTC	Triamcinolone acetonide	1703037	23393	40
Euro OTC	Triamcinolone acetonide	1706013	23557	40
Euro OTC	Triamcinolone acetonide	1710002	23694	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Triamcinolone acetonide	1801020	23883	40
Euro OTC	Triamcinolone acetonide	1805001-01	24191	40
Euro OTC	Triamcinolone acetonide	1810015	24333	40
Euro OTC	Triamcinolone acetonide	1903015	24629	40
Euro OTC	Triamcinolone acetonide	1907044	24842	40
Euro OTC	Triamcinolone acetonide	2001017	25115	40
Euro OTC	Triamcinolone acetonide	2002047	25117	40
Euro OTC	Triamcinolone acetonide	2006032	25456	40
Euro OTC	Triamcinolone acetonide	2012006	25526	40
Euro OTC	Triamcinolone acetonide	2109004	25832	50
Euro OTC	Triamcinolone acetonide	2208004	26261	40
Euro OTC	Triamcinolone acetonide	2308018	26930	40
Fagron	Triamcinolone acetonide	13C13-N20	21043	60
Fagron	Triamcinolone acetonide	22A22-B02-221452	26131	40
Caelo	Triamcinolone acetonide	160945	22473SI	40
Caelo	Triamcinolone acetonide	171206	23330SI	20
Caelo	Triamcinolone acetonide	171206	23343	40
Caelo	Triamcinolone acetonide	171206	23343SI	20
Caelo	Triamcinolone acetonide	181002	24016SI	20
Caelo	Triamcinolone acetonide	190619	24509SI	20
Caelo	Triamcinolone acetonide	23002617	26965SI	30
Euro OTC	Triamcinolone acetonide	1508008	21883SI†	30
Euro OTC	Triamcinolone acetonide	1612014	22978SI	29
Euro OTC	Triamcinolone acetonide	1703037	23393SI	20
Euro OTC	Triamcinolone acetonide	1706013	23557SI	20
Euro OTC	Triamcinolone acetonide	1710002	23694SI	20
Euro OTC	Triamcinolone acetonide	1801020	23883SI	20
Euro OTC	Triamcinolone acetonide	1805001-01	24191SI	20
Euro OTC	Triamcinolone acetonide	1810015	24333SI	20
Euro OTC	Triamcinolone acetonide	1903015	24629SI	20
Euro OTC	Triamcinolone acetonide	1907044	24842SI	20
Euro OTC	Triamcinolone acetonide	2001017	25115SI	40
Euro OTC	Triamcinolone acetonide	2002047	25117SI	20
Euro OTC	Triamcinolone acetonide	2006032	25456SI	20
Euro OTC	Triamcinolone acetonide	2012006	25526SI	20
Euro OTC	Triamcinolone acetonide	2109004	25832SI	30
Euro OTC	Triamcinolone acetonide	2208004	26261SI	30
Euro OTC	Triamcinolone acetonide	2308018	26930SI	31
Fagron	Triamcinolone acetonide	15C19-B06-308572	21962SI†	19
Fagron	Triamcinolone acetonide	22A22-B02-221452	26131SI	30

- 200 405 spectra from a total of 4019 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5559 spectra from 1283 *Apo-Ident* customers from 846 batches from the substance/substance group *Triamcinolone acetonide*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- Among them are spectra of independent samples from 807 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Triamcinolone acetonide	1403009-01	1
	Triamcinolone acetonide	2012006-01	1
	Triamcinolone acetonide	21000116011	1
	Triamcinolone acetonide	21003093011	1
	Triamcinolone acetonide	21003093012	1
	Triamcinolone acetonide	21003093013	3
	Triamcinolone acetonide	2109004-01	2
	Triamcinolone acetonide	2109004-03	2
	Triamcinolone acetonide	21H25-F03-379863	1
	Triamcinolone acetonide	21H25-F03-379875	1
	Triamcinolone acetonide	2200004-01	1
	Triamcinolone acetonide	220000902012	1
	Triamcinolone acetonide	22000902001	3
	Triamcinolone acetonide	22000902002	3
	Triamcinolone acetonide	22000902004	1
	Triamcinolone acetonide	22000902005	4
	Triamcinolone acetonide	22000902008	7
	Triamcinolone acetonide	22000902009	10
	Triamcinolone acetonide	22000902010	6
	Triamcinolone acetonide	22000902012	3
	Triamcinolone acetonide	22000902013	1
	Triamcinolone acetonide	22000902014	2
	Triamcinolone acetonide	22000902015	1
	Triamcinolone acetonide	22000902016	8
	Triamcinolone acetonide	22000902018	7
	Triamcinolone acetonide	22000902019	5
	Triamcinolone acetonide	2200090212	1
	Triamcinolone acetonide	2208004-01	34
	Triamcinolone acetonide	2208004-02	6
	Triamcinolone acetonide	22A22-B01-218005	2
	Triamcinolone acetonide	22A2-BO1-218005	1
	Triamcinolone acetonide	22D15-B01-220144	2
	Triamcinolone acetonide	22D15-B01-222391	2
	Triamcinolone acetonide	22D15-B01-222393	2
	Triamcinolone acetonide	23002018-02	1
	Triamcinolone acetonide	23002073005	1
	Triamcinolone acetonide	23003235001	1
	Triamcinolone acetonide	2305018-01	1
	Triamcinolone acetonide	2308018-01	6
	Triamcinolone acetonide	2308018-02	1
	Triamcinolone acetonide	23C28-B04-227509	1
	Triamcinolone acetonide	NB0601M	2
16804-B07	Triamcinolone acetonide	16B04/B07	1
2001017-0	Triamcinolone acetonide	2001017-01	1
A.H. 07.05.13 ek: 7,25EUR	Triamcinolone acetonide	1211013-02	1
A.H.D.	Triamcinolone acetonide	12301508	1
AHD 03.03.2015	Triamcinolone acetonide	NT1430M	1
AHD 06.03.15 9,47	Triamcinolone acetonide	14355102	2
AHD 17.07.2020	Triamcinolone acetonide	NA0088M	1
AHD 22.12.16 EK 29,74	Triamcinolone acetonide	16D14B11322136	1
AHD/Hedinger	Triamcinolone acetonide	15233902	1
AHD	Triamcinolone acetonide	14355711	1
AHD	Triamcinolone acetonide	17057905	4
AHD	Triamcinolone acetonide	20B28-F04-371546	1
AHD	Triamcinolone acetonide	21003093001	1
AHD	Triamcinolone acetonide	22000902009	1
AHD	Triamcinolone acetonide	22000902018	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
AHD	Triamcinolone acetonide	22000902019	1
AHD	Triamcinolone acetonide	2208004-01	2
AHD	Triamcinolone acetonide	2208004-02	1
AHD	Triamcinolone acetonide	APU0544/315240T	1
AhHD	Triamcinolone acetonide	22000902016	1
Alliance Healthcare	Triamcinolone acetonide	13C13-N20	2
Alliance Healthcare	Triamcinolone acetonide	21000116001	1
Alliance	Triamcinolone acetonide	21003093001	1
Alliance	Triamcinolone acetonide	22000902009	1
Alliance	Triamcinolone acetonide	2208004-01	2
Allianz Healthcare	Triamcinolone acetonide	16080005-01	1
almirall/gehe	Triamcinolone acetonide	17120607	4
Anzag	Triamcinolone acetonide	1303001-02	1
Anzag	Triamcinolone acetonide	14355103	1
Anzag	Triamcinolone acetonide	14355711	1
Anzag	Triamcinolone acetonide	1605010-01	1
Anzag	Triamcinolone acetonide	17120605	1
Anzag	Triamcinolone acetonide	20002630005	1
Anzag	Triamcinolone acetonide	201200601	1
Anzag	Triamcinolone acetonide	2012006-01	1
Anzag	Triamcinolone acetonide	2208004-01	1
apo ident	Triamcinolone acetonide	1612014-01	1
Apo Ident	Triamcinolone acetonide	1907044-01	1
APO III	Triamcinolone acetonide	21003093005	1
apoident	Triamcinolone acetonide	1508008-01	1
apo-ident	Triamcinolone acetonide	1608005-01	1
apo-ident	Triamcinolone acetonide	1801020-01	1
apo-ident	Triamcinolone acetonide	1810015-01	1
apomix	Triamcinolone acetonide	13k15-b31-289029	2
apomix	Triamcinolone acetonide	17120606	2
Apotheke Mildenau	Triamcinolone acetonide	13C13-N20	1
Audor Pharma	Triamcinolone acetonide	15240T	1
Audor Pharma	Triamcinolone acetonide	APNET180403T	3
Audor Pharma	Triamcinolone acetonide	APU0544/315240T	3
Audor Pharma	Triamcinolone acetonide	APU0544/3162705	1
Audor Pharma	Triamcinolone acetonide	APU0544/316270T	2
Audor Pharma	Triamcinolone acetonide	APU0544/317171T	1
Audor Pharma	Triamcinolone acetonide	APU0544/31524T	1
Audor Pharma	Triamcinolone acetonide	U0544/315240T	1
Beiersdorf	Triamcinolone acetonide	18F14-B01-351889	1
Berkel AHK	Triamcinolone acetonide	14355101	3
Bombas/Sanac	Triamcinolone acetonide	16094506	1
Bombastus	Triamcinolone acetonide	13K15-B31	2
Bombastus	Triamcinolone acetonide	17120610	1
Bombastus	Triamcinolone acetonide	1810015-01	1
Cael/Sanacorp	Triamcinolone acetonide	171002-01	1
Caelo	Triamcinolone acetonide	100/AKD2	1
Caelo	Triamcinolone acetonide	10220341	1
Caelo	Triamcinolone acetonide	1040417	1
Caelo	Triamcinolone acetonide	11022021-02	1
Caelo	Triamcinolone acetonide	1107212516	1
Caelo	Triamcinolone acetonide	1110005-01	1
Caelo	Triamcinolone acetonide	1120717/16094502	1
Caelo	Triamcinolone acetonide	11267704	1
Caelo	Triamcinolone acetonide	11267705	1
Caelo	Triamcinolone acetonide	11267707	4
Caelo	Triamcinolone acetonide	11267710	2
Caelo	Triamcinolone acetonide	11267720	1
Caelo	Triamcinolone acetonide	11267721	2
Caelo	Triamcinolone acetonide	116D14B11325479	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triamcinolone acetonide	12/10-N09	3
Caelo	Triamcinolone acetonide	1201506	1
Caelo	Triamcinolone acetonide	1203160l	1
Caelo	Triamcinolone acetonide	1206008-01	1
Caelo	Triamcinolone acetonide	1209040-01	1
Caelo	Triamcinolone acetonide	120904002	1
Caelo	Triamcinolone acetonide	1210-n09	1
Caelo	Triamcinolone acetonide	1211013-01	1
Caelo	Triamcinolone acetonide	12173701	5
Caelo	Triamcinolone acetonide	12173703	1
Caelo	Triamcinolone acetonide	12173704	1
Caelo	Triamcinolone acetonide	12173705	2
Caelo	Triamcinolone acetonide	12173707	5
Caelo	Triamcinolone acetonide	12173710	5
Caelo	Triamcinolone acetonide	12301501	4
Caelo	Triamcinolone acetonide	12301502	1
Caelo	Triamcinolone acetonide	12301503	1
Caelo	Triamcinolone acetonide	12301504	1
Caelo	Triamcinolone acetonide	12301505	1
Caelo	Triamcinolone acetonide	12301506	1
Caelo	Triamcinolone acetonide	12301507	8
Caelo	Triamcinolone acetonide	12301508	4
Caelo	Triamcinolone acetonide	12301509	4
Caelo	Triamcinolone acetonide	12301510	4
Caelo	Triamcinolone acetonide	12301515	12
Caelo	Triamcinolone acetonide	12301518	4
Caelo	Triamcinolone acetonide	1230517/16094502	1
Caelo	Triamcinolone acetonide	1257952	1
Caelo	Triamcinolone acetonide	12E15-N03	1
Caelo	Triamcinolone acetonide	1303001-02	1
Caelo	Triamcinolone acetonide	1312407	1
Caelo	Triamcinolone acetonide	13124801	6
Caelo	Triamcinolone acetonide	13124803	2
Caelo	Triamcinolone acetonide	13124804	14
Caelo	Triamcinolone acetonide	13124805	7
Caelo	Triamcinolone acetonide	13124806	2
Caelo	Triamcinolone acetonide	13124807	12
Caelo	Triamcinolone acetonide	13124808	13
Caelo	Triamcinolone acetonide	13124809	1
Caelo	Triamcinolone acetonide	13124810	2
Caelo	Triamcinolone acetonide	13124811	4
Caelo	Triamcinolone acetonide	13256603	1
Caelo	Triamcinolone acetonide	13256604	6
Caelo	Triamcinolone acetonide	13256607	5
Caelo	Triamcinolone acetonide	13256608	2
Caelo	Triamcinolone acetonide	13379901	1
Caelo	Triamcinolone acetonide	13379903	2
Caelo	Triamcinolone acetonide	13379904	6
Caelo	Triamcinolone acetonide	13379905	19
Caelo	Triamcinolone acetonide	13379906	6
Caelo	Triamcinolone acetonide	13379911	1
Caelo	Triamcinolone acetonide	13379912	10
Caelo	Triamcinolone acetonide	13379913	4
Caelo	Triamcinolone acetonide	13379914	6
Caelo	Triamcinolone acetonide	13379919	1
Caelo	Triamcinolone acetonide	13379921	1
Caelo	Triamcinolone acetonide	13379922	1
Caelo	Triamcinolone acetonide	1355101	1
Caelo	Triamcinolone acetonide	13C13-N20	2
Caelo	Triamcinolone acetonide	13e15-n03	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triamcinolone acetonide	13E15-N03	2
Caelo	Triamcinolone acetonide	13I26-N11	1
Caelo	Triamcinolone acetonide	13K14-B04-289032	1
Caelo	Triamcinolone acetonide	13K14-B04-289033	2
Caelo	Triamcinolone acetonide	13K15-B31-289027	2
Caelo	Triamcinolone acetonide	13K15-B31-289029	1
Caelo	Triamcinolone acetonide	13K15-B31-289031	1
Caelo	Triamcinolone acetonide	14188302	5
Caelo	Triamcinolone acetonide	14188303	4
Caelo	Triamcinolone acetonide	14188304	4
Caelo	Triamcinolone acetonide	14233904	1
Caelo	Triamcinolone acetonide	14255104	1
Caelo	Triamcinolone acetonide	14355101	12
Caelo	Triamcinolone acetonide	14355102	18
Caelo	Triamcinolone acetonide	14355103	12
Caelo	Triamcinolone acetonide	14355104	2
Caelo	Triamcinolone acetonide	14355701	1
Caelo	Triamcinolone acetonide	14355702	11
Caelo	Triamcinolone acetonide	14355703	3
Caelo	Triamcinolone acetonide	14355704	3
Caelo	Triamcinolone acetonide	14355706	1
Caelo	Triamcinolone acetonide	14355708	11
Caelo	Triamcinolone acetonide	14355709	2
Caelo	Triamcinolone acetonide	14355711	9
Caelo	Triamcinolone acetonide	14355712	7
Caelo	Triamcinolone acetonide	14G23_B07_2976618	1
Caelo	Triamcinolone acetonide	14G23-B07-297619	1
Caelo	Triamcinolone acetonide	1504007-01	1
Caelo	Triamcinolone acetonide	1504007-02	1
Caelo	Triamcinolone acetonide	1504007-2	1
Caelo	Triamcinolone acetonide	1508008-01	2
Caelo	Triamcinolone acetonide	1508008-02	1
Caelo	Triamcinolone acetonide	1514Q2516	1
Caelo	Triamcinolone acetonide	15233901	15
Caelo	Triamcinolone acetonide	15233902	29
Caelo	Triamcinolone acetonide	15233903	27
Caelo	Triamcinolone acetonide	15233903-20160615Ma9	1
Caelo	Triamcinolone acetonide	15233904	14
Caelo	Triamcinolone acetonide	15233905	7
Caelo	Triamcinolone acetonide	15233906	17
Caelo	Triamcinolone acetonide	15233908	3
Caelo	Triamcinolone acetonide	15233909	1
Caelo	Triamcinolone acetonide	1530102	1
Caelo	Triamcinolone acetonide	15308613	1
Caelo	Triamcinolone acetonide	15430102	1
Caelo	Triamcinolone acetonide	15430102I-300916/1	1
Caelo	Triamcinolone acetonide	15430103	7
Caelo	Triamcinolone acetonide	15430105	7
Caelo	Triamcinolone acetonide	15430106	5
Caelo	Triamcinolone acetonide	15430107	15
Caelo	Triamcinolone acetonide	15430108	13
Caelo	Triamcinolone acetonide	15C19-B06-308571	1
Caelo	Triamcinolone acetonide	15C19-B06-308573	1
Caelo	Triamcinolone acetonide	15G31-B07-313597	1
Caelo	Triamcinolone acetonide	15G31-B07-314045	1
Caelo	Triamcinolone acetonide	15L21-B03-316123	1
Caelo	Triamcinolone acetonide	15L21-B03-318663	1
Caelo	Triamcinolone acetonide	160102101	1
Caelo	Triamcinolone acetonide	1601021-01	1
Caelo	Triamcinolone acetonide	160501001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triamcinolone acetonide	1605010-01	1
Caelo	Triamcinolone acetonide	16079502	1
Caelo	Triamcinolone acetonide	160800501	1
Caelo	Triamcinolone acetonide	1608005-01	8
Caelo	Triamcinolone acetonide	16092504	24
Caelo	Triamcinolone acetonide	16094501	10
Caelo	Triamcinolone acetonide	16094502	2
Caelo	Triamcinolone acetonide	16094504	6
Caelo	Triamcinolone acetonide	16094505	2
Caelo	Triamcinolone acetonide	16094506	8
Caelo	Triamcinolone acetonide	16094507	5
Caelo	Triamcinolone acetonide	16094511	17
Caelo	Triamcinolone acetonide	16094512	5
Caelo	Triamcinolone acetonide	16094513	1
Caelo	Triamcinolone acetonide	16094514	28
Caelo	Triamcinolone acetonide	1612014	1
Caelo	Triamcinolone acetonide	1612014-01	8
Caelo	Triamcinolone acetonide	16B04-B07-318957	1
Caelo	Triamcinolone acetonide	16D14-B11	1
Caelo	Triamcinolone acetonide	16D14-B11-321318	1
Caelo	Triamcinolone acetonide	16D14-B11-325482	2
Caelo	Triamcinolone acetonide	16D14-B11-328167	1
Caelo	Triamcinolone acetonide	16D16-B11-325482	1
Caelo	Triamcinolone acetonide	16K07-B06-329447	1
Caelo	Triamcinolone acetonide	16K07-B06-332102	1
Caelo	Triamcinolone acetonide	16K07-B06-333438	3
Caelo	Triamcinolone acetonide	17030347-01	1
Caelo	Triamcinolone acetonide	1703037	1
Caelo	Triamcinolone acetonide	170303701	2
Caelo	Triamcinolone acetonide	1703037-01	2
Caelo	Triamcinolone acetonide	170324T1612014-01	1
Caelo	Triamcinolone acetonide	170547902	1
Caelo	Triamcinolone acetonide	17057901	10
Caelo	Triamcinolone acetonide	17057902	19
Caelo	Triamcinolone acetonide	17057903	2
Caelo	Triamcinolone acetonide	17057905	18
Caelo	Triamcinolone acetonide	17057906	16
Caelo	Triamcinolone acetonide	17057907	9
Caelo	Triamcinolone acetonide	17057908	19
Caelo	Triamcinolone acetonide	17057909	2
Caelo	Triamcinolone acetonide	17057910	1
Caelo	Triamcinolone acetonide	1705797	1
Caelo	Triamcinolone acetonide	1706013-01	5
Caelo	Triamcinolone acetonide	17060131	1
Caelo	Triamcinolone acetonide	1706601-01	1
Caelo	Triamcinolone acetonide	1710002-01	1
Caelo	Triamcinolone acetonide	17100201	1
Caelo	Triamcinolone acetonide	1710610	1
Caelo	Triamcinolone acetonide	17120603	25
Caelo	Triamcinolone acetonide	17120604	7
Caelo	Triamcinolone acetonide	17120605	11
Caelo	Triamcinolone acetonide	17120606	21
Caelo	Triamcinolone acetonide	17120606/1211117	1
Caelo	Triamcinolone acetonide	17120607	9
Caelo	Triamcinolone acetonide	17120608	17
Caelo	Triamcinolone acetonide	17120609	1
Caelo	Triamcinolone acetonide	17120610	18
Caelo	Triamcinolone acetonide	17120611	35
Caelo	Triamcinolone acetonide	17120618	6
Caelo	Triamcinolone acetonide	17120619	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triamcinolone acetonide	17120620	11
Caelo	Triamcinolone acetonide	17128606	1
Caelo	Triamcinolone acetonide	1720606	1
Caelo	Triamcinolone acetonide	1720608	1
Caelo	Triamcinolone acetonide	1735302	1
Caelo	Triamcinolone acetonide	17356306	1
Caelo	Triamcinolone acetonide	1735802	1
Caelo	Triamcinolone acetonide	1735805	1
Caelo	Triamcinolone acetonide	17358302	47
Caelo	Triamcinolone acetonide	17358302-T20181115Ma	1
Caelo	Triamcinolone acetonide	17358303	8
Caelo	Triamcinolone acetonide	17358304	14
Caelo	Triamcinolone acetonide	17358305	40
Caelo	Triamcinolone acetonide	17358309	2
Caelo	Triamcinolone acetonide	1738305	1
Caelo	Triamcinolone acetonide	17C09-B01-340173	1
Caelo	Triamcinolone acetonide	17c09-b01-340174	1
Caelo	Triamcinolone acetonide	17C09-B01-340174	2
Caelo	Triamcinolone acetonide	17H03-B12-343457	1
Caelo	Triamcinolone acetonide	17H03-B12-343459	1
Caelo	Triamcinolone acetonide	17H03-B12-345552	1
Caelo	Triamcinolone acetonide	17H03B12346697	1
Caelo	Triamcinolone acetonide	180102001	2
Caelo	Triamcinolone acetonide	1801020-01	6
Caelo	Triamcinolone acetonide	18010202-01	1
Caelo	Triamcinolone acetonide	1805001-01	7
Caelo	Triamcinolone acetonide	180500102	1
Caelo	Triamcinolone acetonide	1805001-02	2
Caelo	Triamcinolone acetonide	1810015-01	2
Caelo	Triamcinolone acetonide	18100203	11
Caelo	Triamcinolone acetonide	18100204	18
Caelo	Triamcinolone acetonide	18100205	14
Caelo	Triamcinolone acetonide	18100206	9
Caelo	Triamcinolone acetonide	18100207	3
Caelo	Triamcinolone acetonide	18100208	10
Caelo	Triamcinolone acetonide	18100209	12
Caelo	Triamcinolone acetonide	18100210	30
Caelo	Triamcinolone acetonide	18100213	28
Caelo	Triamcinolone acetonide	18100215	1
Caelo	Triamcinolone acetonide	18100217	5
Caelo	Triamcinolone acetonide	18100218	4
Caelo	Triamcinolone acetonide	18100220	21
Caelo	Triamcinolone acetonide	18100221	30
Caelo	Triamcinolone acetonide	18100222	23
Caelo	Triamcinolone acetonide	18100225	3
Caelo	Triamcinolone acetonide	18100226	22
Caelo	Triamcinolone acetonide	1810207	1
Caelo	Triamcinolone acetonide	1810299	1
Caelo	Triamcinolone acetonide	1811211	1
Caelo	Triamcinolone acetonide	18C15-B05-347275	1
Caelo	Triamcinolone acetonide	18C15-B05-349087	1
Caelo	Triamcinolone acetonide	18F14-B01-351889	1
Caelo	Triamcinolone acetonide	18F14-B01-352343	1
Caelo	Triamcinolone acetonide	18F14B01355979	1
Caelo	Triamcinolone acetonide	18F14-B01-355979	1
Caelo	Triamcinolone acetonide	18F14-B01-356853	1
Caelo	Triamcinolone acetonide	1903015_01	1
Caelo	Triamcinolone acetonide	1903015-01	1
Caelo	Triamcinolone acetonide	1907044-01	2
Caelo	Triamcinolone acetonide	1912005	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triamcinolone acetonide	191202003	2
Caelo	Triamcinolone acetonide	191202005	28
Caelo	Triamcinolone acetonide	191202006	20
Caelo	Triamcinolone acetonide	191202007	8
Caelo	Triamcinolone acetonide	19120205	1
Caelo	Triamcinolone acetonide	19120205P-191111-2	1
Caelo	Triamcinolone acetonide	19120206	12
Caelo	Triamcinolone acetonide	19120207	35
Caelo	Triamcinolone acetonide	19120208	27
Caelo	Triamcinolone acetonide	19120209	38
Caelo	Triamcinolone acetonide	19120210	22
Caelo	Triamcinolone acetonide	1912021007	1
Caelo	Triamcinolone acetonide	19120211	23
Caelo	Triamcinolone acetonide	1912208	1
Caelo	Triamcinolone acetonide	19J11-F02-367962	1
Caelo	Triamcinolone acetonide	200000461003	1
Caelo	Triamcinolone acetonide	200002630005	1
Caelo	Triamcinolone acetonide	200002630006	2
Caelo	Triamcinolone acetonide	20000461003	19
Caelo	Triamcinolone acetonide	20000461004	21
Caelo	Triamcinolone acetonide	20000461005	20
Caelo	Triamcinolone acetonide	20000461006	9
Caelo	Triamcinolone acetonide	20000461007	18
Caelo	Triamcinolone acetonide	20000461010	1
Caelo	Triamcinolone acetonide	20002360006	1
Caelo	Triamcinolone acetonide	20002630001	4
Caelo	Triamcinolone acetonide	20002630002	7
Caelo	Triamcinolone acetonide	20002630003	1
Caelo	Triamcinolone acetonide	20002630004	1
Caelo	Triamcinolone acetonide	20002630005	36
Caelo	Triamcinolone acetonide	20002630006	12
Caelo	Triamcinolone acetonide	2000263005	1
Caelo	Triamcinolone acetonide	20004422002	2
Caelo	Triamcinolone acetonide	2000461006	1
Caelo	Triamcinolone acetonide	2000461007	1
Caelo	Triamcinolone acetonide	2000464005	1
Caelo	Triamcinolone acetonide	2001017-01	1
Caelo	Triamcinolone acetonide	2006002-01	4
Caelo	Triamcinolone acetonide	2006032-01	1
Caelo	Triamcinolone acetonide	201200601	1
Caelo	Triamcinolone acetonide	2012006-01	4
Caelo	Triamcinolone acetonide	20B28-F04-371546	3
Caelo	Triamcinolone acetonide	20L18-F01-376650	1
Caelo	Triamcinolone acetonide	210000116002	1
Caelo	Triamcinolone acetonide	210000116014	1
Caelo	Triamcinolone acetonide	21000116001	47
Caelo	Triamcinolone acetonide	21000116002	15
Caelo	Triamcinolone acetonide	21000116003	2
Caelo	Triamcinolone acetonide	21000116004	1
Caelo	Triamcinolone acetonide	21000116005	19
Caelo	Triamcinolone acetonide	21000116006	4
Caelo	Triamcinolone acetonide	21000116008	5
Caelo	Triamcinolone acetonide	21000116010	4
Caelo	Triamcinolone acetonide	21000116011	14
Caelo	Triamcinolone acetonide	21000116014	24
Caelo	Triamcinolone acetonide	21000116016	1
Caelo	Triamcinolone acetonide	21000116018	1
Caelo	Triamcinolone acetonide	21000116019	15
Caelo	Triamcinolone acetonide	21000116021	1
Caelo	Triamcinolone acetonide	21000116022	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triamcinolone acetonide	21000118001	1
Caelo	Triamcinolone acetonide	21000166001	1
Caelo	Triamcinolone acetonide	21000428001	1
Caelo	Triamcinolone acetonide	2100116014	1
Caelo	Triamcinolone acetonide	2100303011	1
Caelo	Triamcinolone acetonide	21003090310	1
Caelo	Triamcinolone acetonide	21003093001	26
Caelo	Triamcinolone acetonide	21003093003	11
Caelo	Triamcinolone acetonide	21003093008	7
Caelo	Triamcinolone acetonide	21003093009	1
Caelo	Triamcinolone acetonide	21003093010	7
Caelo	Triamcinolone acetonide	21003093011	15
Caelo	Triamcinolone acetonide	2109004-02	1
Caelo	Triamcinolone acetonide	22000902001	16
Caelo	Triamcinolone acetonide	22000902002	12
Caelo	Triamcinolone acetonide	22000902004	5
Caelo	Triamcinolone acetonide	22000902005	9
Caelo	Triamcinolone acetonide	22000902007	1
Caelo	Triamcinolone acetonide	22000902008	2
Caelo	Triamcinolone acetonide	22000902010	3
Caelo	Triamcinolone acetonide	2208004-01	1
Caelo	Triamcinolone acetonide	2211171	1
Caelo	Triamcinolone acetonide	2449210001161	1
Caelo	Triamcinolone acetonide	2513M02516	1
Caelo	Triamcinolone acetonide	29091806	1
Caelo	Triamcinolone acetonide	3041206	1
Caelo	Triamcinolone acetonide	310320161	1
Caelo	Triamcinolone acetonide	3110120	2
Caelo	Triamcinolone acetonide	31117-1/16094502	1
Caelo	Triamcinolone acetonide	3282	1
Caelo	Triamcinolone acetonide	3340	1
Caelo	Triamcinolone acetonide	42(18100213)	1
Caelo	Triamcinolone acetonide	4613E2516	1
Caelo	Triamcinolone acetonide	5430105	1
Caelo	Triamcinolone acetonide	6051401	1
Caelo	Triamcinolone acetonide	618E-02516	1
Caelo	Triamcinolone acetonide	8681	1
Caelo	Triamcinolone acetonide	9081305	1
Caelo	Triamcinolone acetonide	912020061	1
Caelo	Triamcinolone acetonide	93/AD1	1
Caelo	Triamcinolone acetonide	9364429	2
Caelo	Triamcinolone acetonide	95/AKD34	1
Caelo	Triamcinolone acetonide	I270715-1	1
Caelo	Triamcinolone acetonide	NA0088M	1
Caelo	Triamcinolone acetonide	NS0571M	1
Caelo	Triamcinolone acetonide	NZ0071M	1
Caesar & Loretz / Noweda	Triamcinolone acetonide	191202006	1
Caesar & Loretz /Phönix	Triamcinolone acetonide	21000116014	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	19120207	2
Caesar & Loretz GmbH...	Triamcinolone acetonide	19120210	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	19120208	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	18100221	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	20000461005	2
Caesar & Loretz GmbH...	Triamcinolone acetonide	13379905	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	20000461003	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	17358309	2
Caesar & Loretz GmbH...	Triamcinolone acetonide	20002630006	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	21000116011	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	19120208	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	22000902009	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Triamcinolone acetonide	19120208	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	20000461005	1
Caesar & Loretz GmbH/AEP	Triamcinolone acetonide	21003093001	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	21000116014	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	191202005	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	21000116002	1
Caesar & Loretz GmbH/Gehe	Triamcinolone acetonide	18100210	1
Caesar & Loretz GmbH/Gehe	Triamcinolone acetonide	18100220	1
Caesar & Loretz GmbH/GEHE	Triamcinolone acetonide	21000116002	1
Caesar & Loretz GmbH/Gehe	Triamcinolone acetonide	22000902016	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	19120207	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	21000116002	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	21003093003	2
Caesar & Loretz GmbH/Gö	Triamcinolone acetonide	21003093011	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	19120210	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	19120211	5
Caesar & Loretz GmbH...	Triamcinolone acetonide	20000461007	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	21000116005	2
Caesar & Loretz GmbH...	Triamcinolone acetonide	21000116019	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	21003093010	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	22000902005	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	18100222	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	191202006	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	20000461006	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	20002630006	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	20002630005	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	21000116001	2
Caesar & Loretz GmbH...	Triamcinolone acetonide	21000116022	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	21003093003	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	22000902001	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	18100209	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	20000461005	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	18100210	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	19120211	2
Caesar & Loretz GmbH...	Triamcinolone acetonide	20000461006	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	20000461007	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	21000116008	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	18100210	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	19120207	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	21003093011	1
Caesar & Loretz GmbH/Ph	Triamcinolone acetonide	19120208	1
Caesar & Loretz GmbH/phö	Triamcinolone acetonide	20000461003	2
Caesar & Loretz GmbH...	Triamcinolone acetonide	20002630006	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	18100213	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	20000461007	2
Caesar & Loretz GmbH...	Triamcinolone acetonide	20002630005	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	21000116002	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	21000116014	2
Caesar & Loretz GmbH...	Triamcinolone acetonide	19120207	1
Caesar & Loretz GmbH...	Triamcinolone acetonide	21000116001	2
Caesar & Loretz GmbH...	Triamcinolone acetonide	21003093001	2
Caesar & Loretz GmbH	Triamcinolone acetonide	17057906	1
Caesar & Loretz GmbH	Triamcinolone acetonide	17057907	1
Caesar & Loretz GmbH	Triamcinolone acetonide	17120610	1
Caesar & Loretz GmbH	Triamcinolone acetonide	17358302	1
Caesar & Loretz GmbH	Triamcinolone acetonide	17358305	2
Caesar & Loretz GmbH	Triamcinolone acetonide	17358309	1
Caesar & Loretz GmbH	Triamcinolone acetonide	175358305	1
Caesar & Loretz GmbH	Triamcinolone acetonide	18100203	3
Caesar & Loretz GmbH	Triamcinolone acetonide	18100206	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Triamcinolone acetonide	18100209	1
Caesar & Loretz GmbH	Triamcinolone acetonide	18100210	3
Caesar & Loretz GmbH	Triamcinolone acetonide	18100213	4
Caesar & Loretz GmbH	Triamcinolone acetonide	18100218	1
Caesar & Loretz GmbH	Triamcinolone acetonide	18100220	2
Caesar & Loretz GmbH	Triamcinolone acetonide	18100221	4
Caesar & Loretz GmbH	Triamcinolone acetonide	18100222	5
Caesar & Loretz GmbH	Triamcinolone acetonide	18100226	2
Caesar & Loretz GmbH	Triamcinolone acetonide	1907044-01	1
Caesar & Loretz GmbH	Triamcinolone acetonide	191202005	2
Caesar & Loretz GmbH	Triamcinolone acetonide	191202006	3
Caesar & Loretz GmbH	Triamcinolone acetonide	19120206	4
Caesar & Loretz GmbH	Triamcinolone acetonide	19120207	3
Caesar & Loretz GmbH	Triamcinolone acetonide	19120208	8
Caesar & Loretz GmbH	Triamcinolone acetonide	19120209	8
Caesar & Loretz GmbH	Triamcinolone acetonide	19120210	3
Caesar & Loretz GmbH	Triamcinolone acetonide	19120211	3
Caesar & Loretz GmbH	Triamcinolone acetonide	20000461003	6
Caesar & Loretz GmbH	Triamcinolone acetonide	20000461004	4
Caesar & Loretz GmbH	Triamcinolone acetonide	20000461005	8
Caesar & Loretz GmbH	Triamcinolone acetonide	20000461006	7
Caesar & Loretz GmbH	Triamcinolone acetonide	20000461007	4
Caesar & Loretz GmbH	Triamcinolone acetonide	20002630001	5
Caesar & Loretz GmbH	Triamcinolone acetonide	20002630002	1
Caesar & Loretz GmbH	Triamcinolone acetonide	20002630005	6
Caesar & Loretz GmbH	Triamcinolone acetonide	20002630006	9
Caesar & Loretz GmbH	Triamcinolone acetonide	20004422002	1
Caesar & Loretz GmbH	Triamcinolone acetonide	2002047-01	1
Caesar & Loretz GmbH	Triamcinolone acetonide	2012006-01	2
Caesar & Loretz GmbH	Triamcinolone acetonide	21000116001	22
Caesar & Loretz GmbH	Triamcinolone acetonide	21000116002	14
Caesar & Loretz GmbH	Triamcinolone acetonide	21000116005	4
Caesar & Loretz GmbH	Triamcinolone acetonide	21000116006	2
Caesar & Loretz GmbH	Triamcinolone acetonide	21000116008	6
Caesar & Loretz GmbH	Triamcinolone acetonide	21000116011	4
Caesar & Loretz GmbH	Triamcinolone acetonide	21000116012	1
Caesar & Loretz GmbH	Triamcinolone acetonide	21000116013	2
Caesar & Loretz GmbH	Triamcinolone acetonide	21000116014	14
Caesar & Loretz GmbH	Triamcinolone acetonide	21000116018	4
Caesar & Loretz GmbH	Triamcinolone acetonide	21000116019	6
Caesar & Loretz GmbH	Triamcinolone acetonide	21000116022	1
Caesar & Loretz GmbH	Triamcinolone acetonide	21003093001	9
Caesar & Loretz GmbH	Triamcinolone acetonide	21003093003	4
Caesar & Loretz GmbH	Triamcinolone acetonide	21003093008	9
Caesar & Loretz GmbH	Triamcinolone acetonide	21003093009	1
Caesar & Loretz GmbH	Triamcinolone acetonide	21003093010	2
Caesar & Loretz GmbH	Triamcinolone acetonide	21003093011	3
Caesar & Loretz GmbH	Triamcinolone acetonide	21003093012	1
Caesar & Loretz GmbH	Triamcinolone acetonide	22000902001	6
Caesar & Loretz GmbH	Triamcinolone acetonide	22000902004	3
Caesar & Loretz GmbH	Triamcinolone acetonide	22000902005	2
Caesar & Loretz GmbH	Triamcinolone acetonide	22000902009	5
Caesar & Loretz GmbH	Triamcinolone acetonide	3695669	1
Caesar & Loretz	Triamcinolone acetonide	17057906	1
Caesar & Loretz	Triamcinolone acetonide	18100204	1
Caesar&loretz,Phoenix	Triamcinolone acetonide	11267705	1
Caesar&loretz,Phoenix	Triamcinolone acetonide	12173703	1
Caesar&loretz,Phoenix	Triamcinolone acetonide	12301502	1
Caleo/ Noweda	Triamcinolone acetonide	16092504	1
Caleo/ Noweda	Triamcinolone acetonide	18100213	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caleo/Phönix	Triamcinolone acetonide	21003093010	2
Calo, Hilden/ Phönix	Triamcinolone acetonide	19120208	1
Calo/Sanacorp	Triamcinolone acetonide	16092504	1
Cealo / Phönix / 22...	Triamcinolone acetonide	18100225	1
Cealo/ AHD	Triamcinolone acetonide	18100221	1
Cealo/Jenne	Triamcinolone acetonide	220826(21003093001)	1
Cealo/Phönix	Triamcinolone acetonide	17057901	1
Cealo	Triamcinolone acetonide	1907044-01	1
Cealo	Triamcinolone acetonide	20000461006	1
Cealo	Triamcinolone acetonide	21000116005	1
cesar&lorentz/Phönix	Triamcinolone acetonide	13124801	1
Christal Pharma/Ober...	Triamcinolone acetonide	U0544/113530	1
Crystal Pharma /Ober...	Triamcinolone acetonide	B0544/114010	2
Crystal pharma/ Ober...	Triamcinolone acetonide	U0544/113530	1
Dr. Wolff	Triamcinolone acetonide	1612014-01	1
Ebert & Jacobi	Triamcinolone acetonide	16K07-B06-329445	1
Eigen/Defektur	Triamcinolone acetonide	U0544/113530	1
E-plus	Triamcinolone acetonide	17120610	2
EuRho / 11	Triamcinolone acetonide	2006032-01	1
EuRho / Alliance	Triamcinolone acetonide	2012006-01	1
Eurho / Alliance	Triamcinolone acetonide	2109004-01	1
EuRho / Phoenix	Triamcinolone acetonide	1612014-01	1
EuRho- Phoenix	Triamcinolone acetonide	1710002-01	1
EuRho- Phoenix	Triamcinolone acetonide	1810015-01	2
EuRho/ AHD	Triamcinolone acetonide	1710002-01	1
EuRho/ Phönix	Triamcinolone acetonide	1907044-01	1
EuRho/ Sanacorp	Triamcinolone acetonide	1703037-01	1
EuRho/ Sanacorp	Triamcinolone acetonide	2109004-01	1
EuRho/Noweda	Triamcinolone acetonide	1601021-01	1
EuRho/Noweda	Triamcinolone acetonide	1706013-01	1
EuRho/Noweda	Triamcinolone acetonide	1710002-01	1
Eurho/Noweda	Triamcinolone acetonide	2012006-01	1
EuRho/Phoenix	Triamcinolone acetonide	1403009-02	1
EuRho/Phoenix	Triamcinolone acetonide	2109004-03	1
EuRho/Phönix	Triamcinolone acetonide	1211013-01	1
EuRho/Phönix	Triamcinolone acetonide	1307043-02	1
EuRho/Phönix	Triamcinolone acetonide	1407044-01	1
Eurho/Phönix	Triamcinolone acetonide	2002047-01	1
Eurho/Phönix	Triamcinolone acetonide	201200601	1
EuRho/Px	Triamcinolone acetonide	219004-02	1
Eurho/Sanacorp	Triamcinolone acetonide	1710002-01	1
EuRho/Sanacorp	Triamcinolone acetonide	2006002-01	1
EuRho	Triamcinolone acetonide	110015-01	1
EuRho	Triamcinolone acetonide	1403009-02	1
EuRho	Triamcinolone acetonide	1407044-02	1
EuRho	Triamcinolone acetonide	150800-08-02	1
EuRho	Triamcinolone acetonide	1508008-02	2
EuRho	Triamcinolone acetonide	1703037-01	2
EuRho	Triamcinolone acetonide	1706013-01	2
EuRho	Triamcinolone acetonide	17100002-01	1
EuRho	Triamcinolone acetonide	171000201	1
EuRho	Triamcinolone acetonide	17100201	1
EuRho	Triamcinolone acetonide	180500101	1
Eurho	Triamcinolone acetonide	1805001-02	1
EuRho	Triamcinolone acetonide	1810015-01	1
EuRho	Triamcinolone acetonide	1905015-01	1
EuRho	Triamcinolone acetonide	1907044-01	2
euRho	Triamcinolone acetonide	2006032-01	1
EuRho	Triamcinolone acetonide	2006032-01	2
EuRho	Triamcinolone acetonide	2012006-01	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
EuRho	Triamcinolone acetonide	2012006-02	1
EuRho	Triamcinolone acetonide	NW2518M	1
Euro / Noweda	Triamcinolone acetonide	1612014-01	1
Euro OCT / Krieger	Triamcinolone acetonide	2002047-01	1
Euro OCT / Krieger	Triamcinolone acetonide	2006032-01	1
Euro OTC	Triamcinolone acetonide		5
Euro OTC	Triamcinolone acetonide	1/10002-01	1
Euro OTC	Triamcinolone acetonide	1013I-02516	1
Euro OTC	Triamcinolone acetonide	1110005-01	2
Euro OTC	Triamcinolone acetonide	111005-01	1
Euro OTC	Triamcinolone acetonide	1112023-01	1
Euro OTC	Triamcinolone acetonide	1112023-02	6
Euro OTC	Triamcinolone acetonide	112014-01	1
Euro OTC	Triamcinolone acetonide	11801020-01	1
Euro OTC	Triamcinolone acetonide	1206008-01	5
Euro OTC	Triamcinolone acetonide	1209040-01	4
Euro OTC	Triamcinolone acetonide	1209040-02	2
Euro OTC	Triamcinolone acetonide	1211013-01	4
Euro OTC	Triamcinolone acetonide	1211013-02	9
Euro OTC	Triamcinolone acetonide	121113-02	1
Euro OTC	Triamcinolone acetonide	1234567	1
Euro OTC	Triamcinolone acetonide	12G6008-01	1
Euro OTC	Triamcinolone acetonide	13030001-01	1
Euro OTC	Triamcinolone acetonide	1303001-01	5
Euro OTC	Triamcinolone acetonide	1303001-02	8
Euro OTC	Triamcinolone acetonide	130704301	1
Euro OTC	Triamcinolone acetonide	1307043-01	16
Euro OTC	Triamcinolone acetonide	130704302	1
Euro OTC	Triamcinolone acetonide	1307043-02	14
Euro OTC	Triamcinolone acetonide	1307043-03	1
Euro OTC	Triamcinolone acetonide	14030009-01	2
Euro OTC	Triamcinolone acetonide	14030009-02	1
Euro OTC	Triamcinolone acetonide	1403009-01	7
Euro OTC	Triamcinolone acetonide	1403009-02	13
Euro OTC	Triamcinolone acetonide	1407044-01	9
Euro OTC	Triamcinolone acetonide	1407044-02	15
Euro OTC	Triamcinolone acetonide	140744-02	1
Euro OTC	Triamcinolone acetonide	14120130	1
Euro OTC	Triamcinolone acetonide	141201301	1
Euro OTC	Triamcinolone acetonide	1412013-01	13
Euro OTC	Triamcinolone acetonide	141201302	4
Euro OTC	Triamcinolone acetonide	1412013-02	9
Euro OTC	Triamcinolone acetonide	141213-02	1
Euro OTC	Triamcinolone acetonide	14188304	1
Euro OTC	Triamcinolone acetonide	150400701	2
Euro OTC	Triamcinolone acetonide	1504007-01	10
Euro OTC	Triamcinolone acetonide	1504007-02	17
Euro OTC	Triamcinolone acetonide	15041007-02	1
Euro OTC	Triamcinolone acetonide	15042014A	1
Euro OTC	Triamcinolone acetonide	1508008	1
Euro OTC	Triamcinolone acetonide	1508008-01	17
Euro OTC	Triamcinolone acetonide	150800802	2
Euro OTC	Triamcinolone acetonide	1508008-02	16
Euro OTC	Triamcinolone acetonide	15081701	1
Euro OTC	Triamcinolone acetonide	15111740	1
Euro OTC	Triamcinolone acetonide	15121806	1
Euro OTC	Triamcinolone acetonide	15233904	1
Euro OTC	Triamcinolone acetonide	15233906	2
Euro OTC	Triamcinolone acetonide	15404007-01	1
Euro OTC	Triamcinolone acetonide	15430103	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Triamcinolone acetonide	15121-b03-316123	1
Euro OTC	Triamcinolone acetonide	15L21-B03-316123	2
Euro OTC	Triamcinolone acetonide	1601021-01	32
Euro OTC	Triamcinolone acetonide	1602005-01	1
Euro OTC	Triamcinolone acetonide	160501001	3
Euro OTC	Triamcinolone acetonide	1605010-01	42
Euro OTC	Triamcinolone acetonide	160510-01	1
Euro OTC	Triamcinolone acetonide	1608005	1
Euro OTC	Triamcinolone acetonide	1608005-01	44
Euro OTC	Triamcinolone acetonide	161006T	1
Euro OTC	Triamcinolone acetonide	1612014-01	64
Euro OTC	Triamcinolone acetonide	1612014-014	1
Euro OTC	Triamcinolone acetonide	161214-01	1
Euro OTC	Triamcinolone acetonide	16D14-B11	1
Euro OTC	Triamcinolone acetonide	16D14-B11-322136	1
Euro OTC	Triamcinolone acetonide	170060013-01	1
Euro OTC	Triamcinolone acetonide	17030307-01	1
Euro OTC	Triamcinolone acetonide	1703037	3
Euro OTC	Triamcinolone acetonide	1703037_01	1
Euro OTC	Triamcinolone acetonide	170303701	3
Euro OTC	Triamcinolone acetonide	1703037-01	56
Euro OTC	Triamcinolone acetonide	1706013	1
Euro OTC	Triamcinolone acetonide	170601301	5
Euro OTC	Triamcinolone acetonide	1706013-01	71
Euro OTC	Triamcinolone acetonide	1706079-01	1
Euro OTC	Triamcinolone acetonide	17061406	1
Euro OTC	Triamcinolone acetonide	171000-01	1
Euro OTC	Triamcinolone acetonide	17100002-01	1
Euro OTC	Triamcinolone acetonide	1710002-01	69
Euro OTC	Triamcinolone acetonide	1710002-1	1
Euro OTC	Triamcinolone acetonide	171002-01	2
Euro OTC	Triamcinolone acetonide	171212T/1703037-01	1
Euro OTC	Triamcinolone acetonide	171302-01	1
Euro OTC	Triamcinolone acetonide	171613-01	1
Euro OTC	Triamcinolone acetonide	1801020	3
Euro OTC	Triamcinolone acetonide	180102001	3
Euro OTC	Triamcinolone acetonide	1801020-01	80
Euro OTC	Triamcinolone acetonide	1801020-1	1
Euro OTC	Triamcinolone acetonide	1805001	1
Euro OTC	Triamcinolone acetonide	180500101	3
Euro OTC	Triamcinolone acetonide	1805001-01	43
Euro OTC	Triamcinolone acetonide	180500102	1
Euro OTC	Triamcinolone acetonide	1805001-02	24
Euro OTC	Triamcinolone acetonide	1810015001	1
Euro OTC	Triamcinolone acetonide	181001501	5
Euro OTC	Triamcinolone acetonide	1810015-01	92
Euro OTC	Triamcinolone acetonide	181016181	1
Euro OTC	Triamcinolone acetonide	181020-1	1
Euro OTC	Triamcinolone acetonide	190301501	1
Euro OTC	Triamcinolone acetonide	1903015-01	64
Euro OTC	Triamcinolone acetonide	1903015-15	1
Euro OTC	Triamcinolone acetonide	19030156-01	1
Euro OTC	Triamcinolone acetonide	190601206	1
Euro OTC	Triamcinolone acetonide	190704401	5
Euro OTC	Triamcinolone acetonide	1907044-01	82
Euro OTC	Triamcinolone acetonide	19070744-01	1
Euro OTC	Triamcinolone acetonide	19074401	1
Euro OTC	Triamcinolone acetonide	190744-01	1
Euro OTC	Triamcinolone acetonide	1912014-01	1
Euro OTC	Triamcinolone acetonide	19120209	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Triamcinolone acetonide	20006032-01	1
Euro OTC	Triamcinolone acetonide	2001017	1
Euro OTC	Triamcinolone acetonide	2001017-01	7
Euro OTC	Triamcinolone acetonide	2002047	3
Euro OTC	Triamcinolone acetonide	200204701	5
Euro OTC	Triamcinolone acetonide	2002047-01	49
Euro OTC	Triamcinolone acetonide	20024047-01	1
Euro OTC	Triamcinolone acetonide	200600201	1
Euro OTC	Triamcinolone acetonide	2006002-01	56
Euro OTC	Triamcinolone acetonide	2006002-1	1
Euro OTC	Triamcinolone acetonide	200603201	1
Euro OTC	Triamcinolone acetonide	2006032-01	53
Euro OTC	Triamcinolone acetonide	2006032-31	1
Euro OTC	Triamcinolone acetonide	2012	1
Euro OTC	Triamcinolone acetonide	2012003-01	1
Euro OTC	Triamcinolone acetonide	2012006	2
Euro OTC	Triamcinolone acetonide	2012006_01	1
Euro OTC	Triamcinolone acetonide	201200601	8
Euro OTC	Triamcinolone acetonide	2012006-01	61
Euro OTC	Triamcinolone acetonide	2012006-02	37
Euro OTC	Triamcinolone acetonide	2012006-04	1
Euro OTC	Triamcinolone acetonide	2012006-1	1
Euro OTC	Triamcinolone acetonide	20130912-5	1
Euro OTC	Triamcinolone acetonide	2015006-01	1
Euro OTC	Triamcinolone acetonide	20212006-01	1
Euro OTC	Triamcinolone acetonide	2108004-03	1
Euro OTC	Triamcinolone acetonide	21090004-01	1
Euro OTC	Triamcinolone acetonide	2109001-03	1
Euro OTC	Triamcinolone acetonide	2109004_01	1
Euro OTC	Triamcinolone acetonide	21090040-02	1
Euro OTC	Triamcinolone acetonide	2109004-01	48
Euro OTC	Triamcinolone acetonide	2109004-02	23
Euro OTC	Triamcinolone acetonide	2109004-03	14
Euro OTC	Triamcinolone acetonide	220800401	1
Euro OTC	Triamcinolone acetonide	2208004-01	11
Euro OTC	Triamcinolone acetonide	2208004-02	1
Euro OTC	Triamcinolone acetonide	23061808	1
Euro OTC	Triamcinolone acetonide	26011804	1
Euro OTC	Triamcinolone acetonide	26081405	1
Euro OTC	Triamcinolone acetonide	2772	1
Euro OTC	Triamcinolone acetonide	28041728	1
Euro OTC	Triamcinolone acetonide	2898	1
Euro OTC	Triamcinolone acetonide	29011503	1
Euro OTC	Triamcinolone acetonide	29081501	1
Euro OTC	Triamcinolone acetonide	3022015A	1
Euro OTC	Triamcinolone acetonide	3051402	1
Euro OTC	Triamcinolone acetonide	31101414	1
Euro OTC	Triamcinolone acetonide	5051816	1
Euro OTC	Triamcinolone acetonide	6702020004	1
Euro OTC	Triamcinolone acetonide	6702020010	2
Euro OTC	Triamcinolone acetonide	6702021007	3
Euro OTC	Triamcinolone acetonide	700124	1
Euro OTC	Triamcinolone acetonide	8031803	1
Euro OTC	Triamcinolone acetonide	80616-5	1
Euro OTC	Triamcinolone acetonide	8700	1
Euro OTC	Triamcinolone acetonide	APB0544/112020T	1
Euro OTC	Triamcinolone acetonide	B0544/111404	1
Euro OTC	Triamcinolone acetonide	NV0635M	1
Euro OTC	Triamcinolone acetonide	NW2518M	1
Euro OTC	Triamcinolone acetonide	NX2518M	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Triamcinolone acetonide	NZ032211	1
Euro OTC	Triamcinolone acetonide	PT49	1
Euro/ Anzag	Triamcinolone acetonide	2012006-02	1
euro/ Anzag	Triamcinolone acetonide	3315I02516	1
Euro/Gehe	Triamcinolone acetonide	1612014-01	1
Euro/Gehe	Triamcinolone acetonide	1703037-01	1
Euro/gehe	Triamcinolone acetonide	2012006-01	1
Euro/Krieger	Triamcinolone acetonide	1907044-01	1
Euro/Noweda	Triamcinolone acetonide	161201401	1
Euro/Phönix	Triamcinolone acetonide	1805401	1
Euro/Phönix	Triamcinolone acetonide	1907044	1
Euro/Sanacorp	Triamcinolone acetonide	2006002-01	1
Euro/Sanacorp	Triamcinolone acetonide	2008032-01	1
euro	Triamcinolone acetonide	1211013-02	1
Euro	Triamcinolone acetonide	1303001-02	1
euroct/gehe	Triamcinolone acetonide	1403009	1
euroct/gehe	Triamcinolone acetonide	1403009-02	1
EuroOCT/Gehe	Triamcinolone acetonide	1710002-01	2
Europharm/Otto	Triamcinolone acetonide	1206008-01	1
Europharm/Otto	Triamcinolone acetonide	1209040-02	1
Europharm/Sanacorp	Triamcinolone acetonide	1211013-01	3
Europharm/Sanacorp	Triamcinolone acetonide	B0544/111040	2
Fagron	Triamcinolone acetonide		3
Fagron	Triamcinolone acetonide	11B22-N05	1
Fagron	Triamcinolone acetonide	11K11-N10	6
Fagron	Triamcinolone acetonide	11N11-N10	1
Fagron	Triamcinolone acetonide	12/10-N09	4
Fagron	Triamcinolone acetonide	12/-N09	1
Fagron	Triamcinolone acetonide	120600801	1
Fagron	Triamcinolone acetonide	1210-N09	1
Fagron	Triamcinolone acetonide	12301503	1
Fagron	Triamcinolone acetonide	12B08N01	1
Fagron	Triamcinolone acetonide	12B08-N01	8
Fagron	Triamcinolone acetonide	12E15/N03	1
Fagron	Triamcinolone acetonide	12E15-N03	21
Fagron	Triamcinolone acetonide	12I10-N09	4
Fagron	Triamcinolone acetonide	12l10-N09	3
Fagron	Triamcinolone acetonide	13/26-N11	7
Fagron	Triamcinolone acetonide	13021408	1
Fagron	Triamcinolone acetonide	13121201	1
Fagron	Triamcinolone acetonide	13126-N11	1
Fagron	Triamcinolone acetonide	1326-N11	1
Fagron	Triamcinolone acetonide	13C13-20	1
Fagron	Triamcinolone acetonide	13c13-n20	1
Fagron	Triamcinolone acetonide	13C13-N20	14
Fagron	Triamcinolone acetonide	13C13-N200217/412	1
Fagron	Triamcinolone acetonide	13e15-n03	1
Fagron	Triamcinolone acetonide	13E15N03	3
Fagron	Triamcinolone acetonide	13E15-N03	44
Fagron	Triamcinolone acetonide	13E15-NO3	1
Fagron	Triamcinolone acetonide	13i26-N11	1
Fagron	Triamcinolone acetonide	13I26N11	1
Fagron	Triamcinolone acetonide	13I26-N11	13
Fagron	Triamcinolone acetonide	13I26-N26	1
Fagron	Triamcinolone acetonide	13K14-b04	1
Fagron	Triamcinolone acetonide	13K14-B04	4
Fagron	Triamcinolone acetonide	13k14-B04-289032	1
Fagron	Triamcinolone acetonide	13K14-B04-289032	6
Fagron	Triamcinolone acetonide	13K14-B04-289033	10
Fagron	Triamcinolone acetonide	13K15-B31	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triamcinolone acetonide	13K15-B31-289025	1
Fagron	Triamcinolone acetonide	13K15-B31-289027	6
Fagron	Triamcinolone acetonide	13K15B31289029	1
Fagron	Triamcinolone acetonide	13K15-B31-289029	3
Fagron	Triamcinolone acetonide	13k15-b31-289030	1
Fagron	Triamcinolone acetonide	13K15-B31-289031	6
Fagron	Triamcinolone acetonide	1407044-01	1
Fagron	Triamcinolone acetonide	1412013-01	1
Fagron	Triamcinolone acetonide	14355104	1
Fagron	Triamcinolone acetonide	14355709	1
Fagron	Triamcinolone acetonide	14F30B01	1
Fagron	Triamcinolone acetonide	14F30-B01	2
Fagron	Triamcinolone acetonide	14F30-B01-296287	4
Fagron	Triamcinolone acetonide	14F30-B021-296287	1
Fagron	Triamcinolone acetonide	14G23-B07	1
Fagron	Triamcinolone acetonide	14G23-B07-297618	5
Fagron	Triamcinolone acetonide	14G23-B07-297619	2
Fagron	Triamcinolone acetonide	14G23-B07-297620	7
Fagron	Triamcinolone acetonide	14G23-BO7-297620	1
Fagron	Triamcinolone acetonide	14k14-B05-302887	1
Fagron	Triamcinolone acetonide	14K14-B05-302887	2
Fagron	Triamcinolone acetonide	14K24N-N01	1
Fagron	Triamcinolone acetonide	1508008-02	1
Fagron	Triamcinolone acetonide	1531-07-313596	1
Fagron	Triamcinolone acetonide	15B02-B03	5
Fagron	Triamcinolone acetonide	15B02-B03-303827	2
Fagron	Triamcinolone acetonide	15B02-B03-303828	5
Fagron	Triamcinolone acetonide	15B02-B03-303830	8
Fagron	Triamcinolone acetonide	15BO2-B03-303828	1
Fagron	Triamcinolone acetonide	15C19-B06	1
Fagron	Triamcinolone acetonide	15C19-B06-308571	1
Fagron	Triamcinolone acetonide	15C19-B06-308572	7
Fagron	Triamcinolone acetonide	15C19-B06-308573	9
Fagron	Triamcinolone acetonide	15C19-B06-309194	2
Fagron	Triamcinolone acetonide	15G31B07	2
Fagron	Triamcinolone acetonide	15G31-B07	2
Fagron	Triamcinolone acetonide	15G31-B07-313596	6
Fagron	Triamcinolone acetonide	15G31B07313597	1
Fagron	Triamcinolone acetonide	15G31-B07-313597	6
Fagron	Triamcinolone acetonide	15G31-B07-314045	6
Fagron	Triamcinolone acetonide	15g31-b07-314046	1
Fagron	Triamcinolone acetonide	15G31-B07-314046	4
Fagron	Triamcinolone acetonide	15G31-B07-314047	3
Fagron	Triamcinolone acetonide	15L21-B03	1
Fagron	Triamcinolone acetonide	15L21-B03-316123	8
Fagron	Triamcinolone acetonide	15L21-B03-318663	4
Fagron	Triamcinolone acetonide	16011407	1
Fagron	Triamcinolone acetonide	16014-B12-3231318	1
Fagron	Triamcinolone acetonide	1608005-01	1
Fagron	Triamcinolone acetonide	1612014-01	1
Fagron	Triamcinolone acetonide	16B04	1
Fagron	Triamcinolone acetonide	16B04-B07	4
Fagron	Triamcinolone acetonide	16B04-B07318664	1
Fagron	Triamcinolone acetonide	16B04-B07-318664	7
Fagron	Triamcinolone acetonide	16B04-B07-318957	6
Fagron	Triamcinolone acetonide	16B04-B07-319471	4
Fagron	Triamcinolone acetonide	16B04-Bo7-318664	1
Fagron	Triamcinolone acetonide	16-B07-318664	1
Fagron	Triamcinolone acetonide	16D04-B11-325479	1
Fagron	Triamcinolone acetonide	16D14_B11_328167	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triamcinolone acetonide	16D14-B11	2
Fagron	Triamcinolone acetonide	16D14-B11_322158	1
Fagron	Triamcinolone acetonide	16D14-B11-321318	3
Fagron	Triamcinolone acetonide	16D14-B11-322135	4
Fagron	Triamcinolone acetonide	16D14-B11-322136	9
Fagron	Triamcinolone acetonide	16D14-B11-322158	10
Fagron	Triamcinolone acetonide	16D14B11325479	1
Fagron	Triamcinolone acetonide	16D14-B11-325479	6
Fagron	Triamcinolone acetonide	16D14-B11-325480	3
Fagron	Triamcinolone acetonide	16D14-B11-325481	1
Fagron	Triamcinolone acetonide	16D14-B11-325482	7
Fagron	Triamcinolone acetonide	16D14-B11-328167	14
Fagron	Triamcinolone acetonide	16K07-B06	3
Fagron	Triamcinolone acetonide	16K07-B060921	1
Fagron	Triamcinolone acetonide	16K07B06329445	1
Fagron	Triamcinolone acetonide	16K07-B06-329445	5
Fagron	Triamcinolone acetonide	16K07-B06-329446	1
Fagron	Triamcinolone acetonide	16K07-B06-329447	1
Fagron	Triamcinolone acetonide	16K07-B06-332101	7
Fagron	Triamcinolone acetonide	16K07-B06-332102	4
Fagron	Triamcinolone acetonide	16k07-b06332103	1
Fagron	Triamcinolone acetonide	16K07B06332103	1
Fagron	Triamcinolone acetonide	16K07-B06-332103	2
Fagron	Triamcinolone acetonide	16K07-B06-333438	4
Fagron	Triamcinolone acetonide	16107-b06-332102	1
Fagron	Triamcinolone acetonide	1703-B12-345553	1
Fagron	Triamcinolone acetonide	17C09_B01_337464	1
Fagron	Triamcinolone acetonide	17C09-B01	3
Fagron	Triamcinolone acetonide	17C09-B01_337464	1
Fagron	Triamcinolone acetonide	17C09-B01-334196	6
Fagron	Triamcinolone acetonide	17C09-B01-334197	4
Fagron	Triamcinolone acetonide	17C-09-B01-334197	1
Fagron	Triamcinolone acetonide	17C09-B01-336881	2
Fagron	Triamcinolone acetonide	17C09-B01-337464	3
Fagron	Triamcinolone acetonide	17C09-B01-340173	10
Fagron	Triamcinolone acetonide	17c09-b01-340174	1
Fagron	Triamcinolone acetonide	17C09-B01-340174	10
Fagron	Triamcinolone acetonide	17C-B01-336881	2
Fagron	Triamcinolone acetonide	17F14-B01-352343	1
Fagron	Triamcinolone acetonide	17H03-812-346697	1
Fagron	Triamcinolone acetonide	17H03-B12	6
Fagron	Triamcinolone acetonide	17H03-B12-343457	6
Fagron	Triamcinolone acetonide	17H03-B12343458	1
Fagron	Triamcinolone acetonide	17H03-B12-343458	6
Fagron	Triamcinolone acetonide	17H03-B12-343459	3
Fagron	Triamcinolone acetonide	17h03-b12-343672	1
Fagron	Triamcinolone acetonide	17H03-B12-343672	6
Fagron	Triamcinolone acetonide	17H03-B12-345552	10
Fagron	Triamcinolone acetonide	17H03-B12-345553	2
Fagron	Triamcinolone acetonide	17H03-B12-346697	2
Fagron	Triamcinolone acetonide	17H03-B12-672	1
Fagron	Triamcinolone acetonide	1810015-01	1
Fagron	Triamcinolone acetonide	18100205	1
Fagron	Triamcinolone acetonide	18100221	1
Fagron	Triamcinolone acetonide	18C15-B05	6
Fagron	Triamcinolone acetonide	18C15-B05_348063	1
Fagron	Triamcinolone acetonide	18C15B05347275	2
Fagron	Triamcinolone acetonide	18C15-B05-347275	6
Fagron	Triamcinolone acetonide	18C15-B05-348063	6
Fagron	Triamcinolone acetonide	18c15-b05-348064	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triamcinolone acetonide	18C15-B05-348064	3
Fagron	Triamcinolone acetonide	18c15-b05-349087	1
Fagron	Triamcinolone acetonide	18C15-B05-349087	8
Fagron	Triamcinolone acetonide	18c15-b05-350263	1
Fagron	Triamcinolone acetonide	18C15-B05-350263	4
Fagron	Triamcinolone acetonide	18C15-B05-348063	1
Fagron	Triamcinolone acetonide	18F14	1
Fagron	Triamcinolone acetonide	18F14_B01_352343	1
Fagron	Triamcinolone acetonide	18F14_B01_352630	1
Fagron	Triamcinolone acetonide	18F14-B01	3
Fagron	Triamcinolone acetonide	18F14-B01_356853	1
Fagron	Triamcinolone acetonide	18f14b01351889	1
Fagron	Triamcinolone acetonide	18F14-B01-351889	7
Fagron	Triamcinolone acetonide	18F14-B01-352343	10
Fagron	Triamcinolone acetonide	18F14-B01-352630	5
Fagron	Triamcinolone acetonide	18F14-B01-353255	9
Fagron	Triamcinolone acetonide	18F14-B01-355724	4
Fagron	Triamcinolone acetonide	18F14-B01-355979	5
Fagron	Triamcinolone acetonide	18F14-B01-356853	13
Fagron	Triamcinolone acetonide	18f14-b01-357073	1
Fagron	Triamcinolone acetonide	18F14-B01-357073	6
Fagron	Triamcinolone acetonide	18F14-B-351889	1
Fagron	Triamcinolone acetonide	18F14-B01-357073	1
Fagron	Triamcinolone acetonide	18I216-B05-361518	1
Fagron	Triamcinolone acetonide	18k16-B05	1
Fagron	Triamcinolone acetonide	18K16-B05	5
Fagron	Triamcinolone acetonide	18K-16-B05	1
Fagron	Triamcinolone acetonide	18K16-B05_367959	1
Fagron	Triamcinolone acetonide	18K16-B05-357775	4
Fagron	Triamcinolone acetonide	18K16-B05-35969	1
Fagron	Triamcinolone acetonide	18K16-B05-359867	7
Fagron	Triamcinolone acetonide	18K16-B05-359868	6
Fagron	Triamcinolone acetonide	18K16-B05-359869	4
Fagron	Triamcinolone acetonide	18K16-B05-359871	8
Fagron	Triamcinolone acetonide	18K16-B05-361518	6
Fagron	Triamcinolone acetonide	18K16-B05-361521	8
Fagron	Triamcinolone acetonide	18K16-B05-361522	2
Fagron	Triamcinolone acetonide	18K-16-B05-361522	1
Fagron	Triamcinolone acetonide	18k16b05361523	1
Fagron	Triamcinolone acetonide	18k16-b05-361523	1
Fagron	Triamcinolone acetonide	18K16-B05-361523	3
Fagron	Triamcinolone acetonide	18K16-B05-367959	5
Fagron	Triamcinolone acetonide	18K16-B06-357775	1
Fagron	Triamcinolone acetonide	19J11-F02	2
Fagron	Triamcinolone acetonide	19J11-F02-367958	1
Fagron	Triamcinolone acetonide	19J11-F02367961	1
Fagron	Triamcinolone acetonide	19J11-F02-367961	2
Fagron	Triamcinolone acetonide	19J11-F02-367962	6
Fagron	Triamcinolone acetonide	19J11-F02-368619	1
Fagron	Triamcinolone acetonide	19J11-F02-367958	1
Fagron	Triamcinolone acetonide	19J-F02-367962	1
Fagron	Triamcinolone acetonide	20031302	1
Fagron	Triamcinolone acetonide	20828-F04-371546	1
Fagron	Triamcinolone acetonide	20B28-F04	5
Fagron	Triamcinolone acetonide	20B28-F04-0005	1
Fagron	Triamcinolone acetonide	20B28-F04-3715406	1
Fagron	Triamcinolone acetonide	20B28-F04-371541	7
Fagron	Triamcinolone acetonide	20B28-F04-371542	1
Fagron	Triamcinolone acetonide	20B28F04-371544	1
Fagron	Triamcinolone acetonide	20B28-F04-371544	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triamcinolone acetonide	20b28-f04-371546	1
Fagron	Triamcinolone acetonide	20b28-F04-371546	1
Fagron	Triamcinolone acetonide	20B28-F04-371546	15
Fagron	Triamcinolone acetonide	20L18-F01	3
Fagron	Triamcinolone acetonide	20L-18-F01	1
Fagron	Triamcinolone acetonide	20l18-f01-376647	1
Fagron	Triamcinolone acetonide	20L18-F01-376647	7
Fagron	Triamcinolone acetonide	20L18-F01-376649	2
Fagron	Triamcinolone acetonide	20L18-F01-376650	8
Fagron	Triamcinolone acetonide	20L18-F01-376653	1
Fagron	Triamcinolone acetonide	20L18F01-376658	1
Fagron	Triamcinolone acetonide	20L18-F01-376658	3
Fagron	Triamcinolone acetonide	20L18FO1376658	1
Fagron	Triamcinolone acetonide	21H04-B13-21363	1
Fagron	Triamcinolone acetonide	21H04-B13-213632	1
Fagron	Triamcinolone acetonide	21H04-B13-213633	3
Fagron	Triamcinolone acetonide	21H25-F03-379863	5
Fagron	Triamcinolone acetonide	21H25-F03-379867	7
Fagron	Triamcinolone acetonide	21H25-F03-379871	3
Fagron	Triamcinolone acetonide	21H25-F03-379874	15
Fagron	Triamcinolone acetonide	21H25-F03-379875	13
Fagron	Triamcinolone acetonide	21H25-FO3-379871	1
Fagron	Triamcinolone acetonide	21J20-B03	2
Fagron	Triamcinolone acetonide	21j20-b03-217884	1
Fagron	Triamcinolone acetonide	21J20-B03-217884	7
Fagron	Triamcinolone acetonide	21J20-Bo3-217884	1
Fagron	Triamcinolone acetonide	21J20-BO3-217884	1
Fagron	Triamcinolone acetonide	22A22-B01-218005	2
Fagron	Triamcinolone acetonide	22A22-B01-218005/NB3123M	1
Fagron	Triamcinolone acetonide	22D15-B01-220144	2
Fagron	Triamcinolone acetonide	289027	1
Fagron	Triamcinolone acetonide	3212U-02516(NP)	1
Fagron	Triamcinolone acetonide	355724	1
Fagron	Triamcinolone acetonide	411082-1-P	1
Fagron	Triamcinolone acetonide	4111408	1
Fagron	Triamcinolone acetonide	5061205	1
Fagron	Triamcinolone acetonide	5061303	1
Fagron	Triamcinolone acetonide	5121302	1
Fagron	Triamcinolone acetonide	7041501	1
Fagron	Triamcinolone acetonide	9041305	1
Fagron	Triamcinolone acetonide	B05-3480603	1
Fagron	Triamcinolone acetonide	B05-3598607	1
Fagron	Triamcinolone acetonide	B053679509	1
Fagron	Triamcinolone acetonide	C22H25CIN209	1
Fagron	Triamcinolone acetonide	F01_3766500	1
Fagron	Triamcinolone acetonide	F01-3766407	1
Fagron	Triamcinolone acetonide	F01-3766507	1
Fagron	Triamcinolone acetonide	F01-3766508	1
Fagron	Triamcinolone acetonide	F01-376653	1
Fagron	Triamcinolone acetonide	F02-3679508	1
Fagron	Triamcinolone acetonide	F02-3679602	1
Fagron	Triamcinolone acetonide	F03-3798603	1
Fagron	Triamcinolone acetonide	F03-3798704	1
Fagron	Triamcinolone acetonide	F04-3715401	1
Fagron	Triamcinolone acetonide	F04-3715406	5
Fagron	Triamcinolone acetonide	F08-3679508	1
Fagron	Triamcinolone acetonide	FO1-3766507	1
Fagron	Triamcinolone acetonide	NA0087M	3
Fagron	Triamcinolone acetonide	NA3552M	6
Fagron	Triamcinolone acetonide	NB0601M	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triamcinolone acetonide	NBO601M	2
Fagron	Triamcinolone acetonide	NS0571M	5
Fagron	Triamcinolone acetonide	NS0996M	2
Fagron	Triamcinolone acetonide	NS2236M	1
Fagron	Triamcinolone acetonide	NSO571M	1
Fagron	Triamcinolone acetonide	NT0487M	1
Fagron	Triamcinolone acetonide	NT0770M	1
Fagron	Triamcinolone acetonide	NT077oM	1
Fagron	Triamcinolone acetonide	NT1094M	1
Fagron	Triamcinolone acetonide	NT1430M	3
Fagron	Triamcinolone acetonide	NU0930M	1
Fagron	Triamcinolone acetonide	NVO262M	1
Fagron	Triamcinolone acetonide	Nw0635M	1
Fagron	Triamcinolone acetonide	NW2261M	2
Fagron	Triamcinolone acetonide	NW2518M	1
Fagron	Triamcinolone acetonide	NX0241M	1
Fagron	Triamcinolone acetonide	NX1540M	2
Fagron	Triamcinolone acetonide	ny0485m	1
Fagron	Triamcinolone acetonide	NY0485M	5
Fagron	Triamcinolone acetonide	NY1271M	6
Fagron	Triamcinolone acetonide	NY2097M	2
Fargon / AHD	Triamcinolone acetonide	18C15-B05-350263	1
Fargon/Alliance HC	Triamcinolone acetonide	15B02-B03-303830	1
Fargon/Anzag	Triamcinolone acetonide	13/26-N11	3
Fargon/Gehe	Triamcinolone acetonide	16D14-B11	1
Fargon/Phoenix	Triamcinolone acetonide	18K16-B05-359871	1
fargon	Triamcinolone acetonide	13C13-N20	1
Fargon	Triamcinolone acetonide	15C19-B06-308572	2
Fargon	Triamcinolone acetonide	15C19-B06-308573	1
Fargon	Triamcinolone acetonide	Nu2526M	1
Fargron	Triamcinolone acetonide	13/26-N11	1
Farmabios / Gehe	Triamcinolone acetonide	15233905	1
Farmabios S.p.A. IT	Triamcinolone acetonide	18100213	1
Farmabios S.p.A./Cae…	Triamcinolone acetonide	15233901	1
Fiebig	Triamcinolone acetonide	15C19-B06-308571	1
Fiebig	Triamcinolone acetonide	16B04-B07-318957	1
Fiebig	Triamcinolone acetonide	17057902	1
Fiebig	Triamcinolone acetonide	1805001-02	1
Fiebig	Triamcinolone acetonide	20000461004	1
Finteler Apotheke	Triamcinolone acetonide	17057910	1
fragon/phonix	Triamcinolone acetonide	18K16-B05-357636	1
Fragon	Triamcinolone acetonide	21H25-F03-379867	1
Fragron/ Alliance	Triamcinolone acetonide	20L-18-F01-376658	1
Gehe amax	Triamcinolone acetonide	17C09-B01-340174	1
Gehe amax	Triamcinolone acetonide	1801020-01	1
Gehe amax	Triamcinolone acetonide	1903015-01	1
Gehe Apo-ident	Triamcinolone acetonide	201200601	1
Gehe Rostock	Triamcinolone acetonide	19120211	1
Gehe Rostock	Triamcinolone acetonide	21000116019	1
Gehe Rostock	Triamcinolone acetonide	2100016019	1
Gehe/EuRo	Triamcinolone acetonide	1605010-01	1
Gehe/EuRo	Triamcinolone acetonide	1801020-01	1
Gehe/EuRoh	Triamcinolone acetonide	2006002-01	1
Gehe/Fragon	Triamcinolone acetonide	16D14-B11-325479	1
Gehe/Phönix	Triamcinolone acetonide	1209040-02	1
Gehe	Triamcinolone acetonide	12/10-N09	2
Gehe	Triamcinolone acetonide	12301510	2
Gehe	Triamcinolone acetonide	12E15-N03	1
Gehe	Triamcinolone acetonide	13124805	1
Gehe	Triamcinolone acetonide	13E15-N03	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Triamcinolone acetonide	13I26-N11	1
Gehe	Triamcinolone acetonide	1504007-01	1
Gehe	Triamcinolone acetonide	15430102	2
Gehe	Triamcinolone acetonide	15B02-B03-303827	1
GEHE	Triamcinolone acetonide	1605010-01	1
Gehe	Triamcinolone acetonide	160800501	1
Gehe	Triamcinolone acetonide	1608005-01	1
Gehe	Triamcinolone acetonide	16094501	1
Gehe	Triamcinolone acetonide	1612014-01	1
GEHE	Triamcinolone acetonide	16K07-B06-332103	1
Gehe	Triamcinolone acetonide	1703037	1
Gehe	Triamcinolone acetonide	170601301	1
Gehe	Triamcinolone acetonide	1706013-01	2
GEHE	Triamcinolone acetonide	1706013-01	1
Gehe	Triamcinolone acetonide	1710002-01	1
GEHE	Triamcinolone acetonide	1710002-01	1
Gehe	Triamcinolone acetonide	17120606	2
Gehe	Triamcinolone acetonide	17120610	1
GEHE	Triamcinolone acetonide	17358303	1
Gehe	Triamcinolone acetonide	1801020-01	1
Gehe	Triamcinolone acetonide	1805001-01	1
Gehe	Triamcinolone acetonide	1805001-02	1
Gehe	Triamcinolone acetonide	1810015-01	2
GEHE	Triamcinolone acetonide	1810015-01	1
Gehe	Triamcinolone acetonide	18100203	1
Gehe	Triamcinolone acetonide	18100206	1
GEHE	Triamcinolone acetonide	18100206	1
Gehe	Triamcinolone acetonide	18100208	2
Gehe	Triamcinolone acetonide	18100222	1
GEHE	Triamcinolone acetonide	18100225	2
Gehe	Triamcinolone acetonide	18C15-B05	1
Gehe	Triamcinolone acetonide	18K16-B05-367959	1
Gehe	Triamcinolone acetonide	1903015-01	3
Gehe	Triamcinolone acetonide	1903018-01	1
Gehe	Triamcinolone acetonide	19J11-F02	1
Gehe	Triamcinolone acetonide	20000461003	1
Gehe	Triamcinolone acetonide	20000461004	1
Gehe	Triamcinolone acetonide	2001017-01	1
Gehe	Triamcinolone acetonide	2012006-01	1
Gehe	Triamcinolone acetonide	20B28F04371542	1
Gehe	Triamcinolone acetonide	21000116001	2
Gehe	Triamcinolone acetonide	21000116005	1
Gehe	Triamcinolone acetonide	21000116014	1
Gehe	Triamcinolone acetonide	2109004-03	1
Gehe	Triamcinolone acetonide	21H25-F03-379875	1
Gehe	Triamcinolone acetonide	22000902005	1
GEHE	Triamcinolone acetonide	22000902012	1
gehe	Triamcinolone acetonide	22000902019	1
gehe	Triamcinolone acetonide	2200902019	1
Gehe	Triamcinolone acetonide	2208004-01	3
GEHE	Triamcinolone acetonide	2208004-02	1
Gehe	Triamcinolone acetonide	22A22-B01-218005	3
Gehe	Triamcinolone acetonide	700124-0007	1
Geibo/ Fargron	Triamcinolone acetonide	16D14-B11-322158	1
Geilenkirchen	Triamcinolone acetonide	18K16-B05-357775	1
Geilenkirchen	Triamcinolone acetonide	20000461007	1
Geilenkirchen	Triamcinolone acetonide	21000116008	1
Hirsch	Triamcinolone acetonide	12I10-N09	2
Ichtyol/Gehe	Triamcinolone acetonide	15430102	3
Jenne	Triamcinolone acetonide	1805001-01	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Jenne	Triamcinolone acetonide	18C15-B05-347275	1
Jenne	Triamcinolone acetonide	2012006-01	1
Jenne	Triamcinolone acetonide	21000116001	1
Jenne	Triamcinolone acetonide	2109004-01	2
Jenne	Triamcinolone acetonide	22000902019	2
Jenne	Triamcinolone acetonide	2208004-01	1
Kehr	Triamcinolone acetonide	1057902	1
Kehr	Triamcinolone acetonide	21003093005	1
Kehr	Triamcinolone acetonide	22000902005	1
Kehr	Triamcinolone acetonide	22000902019	1
Kehr	Triamcinolone acetonide	2200902014	1
Kehr	Triamcinolone acetonide	22A22-B01-218005	1
Klenk	Triamcinolone acetonide	1504007-02	1
Klenk	Triamcinolone acetonide	NS1680M	1
Lamotte	Triamcinolone acetonide	19120207	1
Martinus-Apotheke	Triamcinolone acetonide	13379905	1
Midas Göttingen	Triamcinolone acetonide	16094504	1
Midas	Triamcinolone acetonide	16094511	1
Midas	Triamcinolone acetonide	17H03-B12-343457	1
Newchem / Gehe	Triamcinolone acetonide	18F14-B01-355979	1
Newchem / Gehe	Triamcinolone acetonide	191202005	1
Newchem / Gehe	Triamcinolone acetonide	B05-3598701	1
Newchem / Gehe	Triamcinolone acetonide	NV2998M	1
NEWCHEM / Sanacorp	Triamcinolone acetonide	15040007-01	1
Newchem S. p. A. / Noweda	Triamcinolone acetonide	17120608	1
Newchem S.p.A./Caesa…	Triamcinolone acetonide	1543015	1
NEWCHEM S.P.A.	Triamcinolone acetonide	NV0994M	1
Newchem S.P.A/Allian…	Triamcinolone acetonide	2006032-01	1
Newchem S.P.A	Triamcinolone acetonide	1508008-02	1
Newchem Spa (site)	Triamcinolone acetonide	16K07-B06-332102	1
Newchem Spa	Triamcinolone acetonide	191202006	1
Newchem Spa	Triamcinolone acetonide	19J11-F02-367962	1
Newchem/ Jenne	Triamcinolone acetonide	18F14-B01-356853	1
Newchem/ Noweda	Triamcinolone acetonide	1403009-01	1
Newchem/AHD	Triamcinolone acetonide	1407044-02	1
Newchem/Fiebig	Triamcinolone acetonide	1605010-01	1
Newchem/Kehr	Triamcinolone acetonide	1407044-01	1
Newchem/Noweda	Triamcinolone acetonide	15C19-B06-308573	1
Newchem/Noweda	Triamcinolone acetonide	NA3551M	1
Newchem/Noweda	Triamcinolone acetonide	NZ0071M	2
Newchem/Noweda	Triamcinolone acetonide	NZ3279M	1
Newchem/Phönix	Triamcinolone acetonide	1810015-01	1
Newchem	Triamcinolone acetonide	1303001-02	1
Noveda	Triamcinolone acetonide	12301518	1
Noweda/ NEWCHEM	Triamcinolone acetonide	1211013-02	1
Noweda/Fargon	Triamcinolone acetonide	18K16-B05-359868	1
Noweda	Triamcinolone acetonide	1112023-02	1
Noweda	Triamcinolone acetonide	12301501	1
Noweda	Triamcinolone acetonide	12301509	1
Noweda	Triamcinolone acetonide	12E15-N03	1
noweda	Triamcinolone acetonide	13256604	1
Noweda	Triamcinolone acetonide	13K15-B31-289029	1
Noweda	Triamcinolone acetonide	1407044-01	1
Noweda	Triamcinolone acetonide	14355103	1
Noweda	Triamcinolone acetonide	14355708	1
Noweda	Triamcinolone acetonide	15233902	1
Noweda	Triamcinolone acetonide	15233903	1
Noweda	Triamcinolone acetonide	1605010-01	1
Noweda	Triamcinolone acetonide	1608005-01	1
Noweda	Triamcinolone acetonide	16094514	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Triamcinolone acetonide	1703037-01	4
Noweda	Triamcinolone acetonide	17057905	2
Noweda	Triamcinolone acetonide	17057908	1
Noweda	Triamcinolone acetonide	1706013-01	1
Noweda	Triamcinolone acetonide	17120603	1
Noweda	Triamcinolone acetonide	17120606	2
Noweda	Triamcinolone acetonide	17120611	1
Noweda	Triamcinolone acetonide	17358305	2
Noweda	Triamcinolone acetonide	17H03-B12-343457	1
Noweda	Triamcinolone acetonide	1805001-01	1
Noweda	Triamcinolone acetonide	181000226	1
Noweda	Triamcinolone acetonide	1810015-01	2
Noweda	Triamcinolone acetonide	18100210	2
Noweda	Triamcinolone acetonide	18100213	1
Noweda	Triamcinolone acetonide	18100221	1
Noweda	Triamcinolone acetonide	18100222	2
Noweda	Triamcinolone acetonide	18K16B05359867	1
Noweda	Triamcinolone acetonide	1903015-01	1
Noweda	Triamcinolone acetonide	1907044-01	1
Noweda	Triamcinolone acetonide	191202005	1
Noweda	Triamcinolone acetonide	19120211	1
Noweda	Triamcinolone acetonide	2006032-01	1
Noweda	Triamcinolone acetonide	2012006-01	1
Noweda	Triamcinolone acetonide	21000116014	1
Noweda	Triamcinolone acetonide	21000116022	1
Noweda	Triamcinolone acetonide	21003093001	1
Noweda	Triamcinolone acetonide	2109004-02	1
Noweda	Triamcinolone acetonide	21H25-F03-379863	1
Noweda	Triamcinolone acetonide	2200902018	1
Noweda	Triamcinolone acetonide	2208004-01	4
Noweda	Triamcinolone acetonide	F04-3715401	1
Noweda	Triamcinolone acetonide	FO4-3715401	1
Noweda	Triamcinolone acetonide	NZ1748M	1
Oberlinden Apotheke	Triamcinolone acetonide	B0544/114010	1
Oberlinden- Apotheke	Triamcinolone acetonide	U0544/113530	1
Oberlinden-Apotheke	Triamcinolone acetonide	U0544/1	1
Parthe Apotheke	Triamcinolone acetonide	55/21	1
Pharmachem/Phönix	Triamcinolone acetonide	1907044-01	1
Phoenix /Eu Rho	Triamcinolone acetonide	2006002-01	1
Phoenix 07.03.2017 11,62EUR	Triamcinolone acetonide	16D14-B11-325480	1
Phoenix 12.03.2019 11,43EUR	Triamcinolone acetonide	18F14-B01-352630	1
Phoenix WE 16.03.17 ...	Triamcinolone acetonide	1612014-01	1
Phoenix,Eu Rho	Triamcinolone acetonide	2208004-01	3
Phoenix	Triamcinolone acetonide	13126-N11	2
Phoenix	Triamcinolone acetonide	14355708	1
Phoenix	Triamcinolone acetonide	14355709	1
Phoenix	Triamcinolone acetonide	1703037	1
Phoenix	Triamcinolone acetonide	1703037-01	1
Phoenix	Triamcinolone acetonide	17057908	2
Phoenix	Triamcinolone acetonide	1706013-01	4
Phoenix	Triamcinolone acetonide	17120603	2
Phoenix	Triamcinolone acetonide	1805001-01	1
Phoenix	Triamcinolone acetonide	18100221	1
Phoenix	Triamcinolone acetonide	2012006-01	1
Phoenix	Triamcinolone acetonide	2012006-02	1
Phoenix	Triamcinolone acetonide	2109004-02	1
Phoenix	Triamcinolone acetonide	21H25-F03_379875	1
Phoenix	Triamcinolone acetonide	22000902008	1
Phoenix	Triamcinolone acetonide	22000902019	1
Phoenix	Triamcinolone acetonide	3064	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Triamcinolone acetonide	3129	1
Phoenix	Triamcinolone acetonide	3219	1
Phoenix	Triamcinolone acetonide	3424	1
Phoenix_25.01.2019	Triamcinolone acetonide	1810015-01	2
phoenix-06.11.18	Triamcinolone acetonide	1801020-01	1
Phönix Gotha	Triamcinolone acetonide	14355711	1
Phönix Gotha	Triamcinolone acetonide	17120610	1
Phönix Gotha	Triamcinolone acetonide	191202005	1
Phönix W.E: 16.04.20...	Triamcinolone acetonide	1710002-01	1
Phönix/Apo-Ident	Triamcinolone acetonide	6702021007	1
Phönix/Caesar&Lorenz...	Triamcinolone acetonide	21003093001	1
Phönix	Triamcinolone acetonide	12E15-N03	1
Phönix	Triamcinolone acetonide	13379902	1
Phönix	Triamcinolone acetonide	13E15-N03	1
Phönix	Triamcinolone acetonide	13K15-B31-289027	1
Phönix	Triamcinolone acetonide	1403009-01	1
Phönix	Triamcinolone acetonide	1407044-01	1
phönix	Triamcinolone acetonide	15233906	1
phönix	Triamcinolone acetonide	15430107	1
phönix	Triamcinolone acetonide	1605010-01	1
Phönix	Triamcinolone acetonide	1608005-01	1
Phönix	Triamcinolone acetonide	17057908	2
Phönix	Triamcinolone acetonide	1706013-01	1
Phönix	Triamcinolone acetonide	1801020-01	1
Phönix	Triamcinolone acetonide	1805001-02	1
Phönix	Triamcinolone acetonide	1810015-01	2
Phönix	Triamcinolone acetonide	18100204	1
Phönix	Triamcinolone acetonide	18F14-B01-032343	1
Phönix	Triamcinolone acetonide	18K16-B05-359871	2
Phönix	Triamcinolone acetonide	18K16-B05-361521	1
Phönix	Triamcinolone acetonide	1903015	1
Phönix	Triamcinolone acetonide	1907044-01	1
Phönix	Triamcinolone acetonide	19120207	1
Phönix	Triamcinolone acetonide	19120209	1
Phönix	Triamcinolone acetonide	19120210	1
Phönix	Triamcinolone acetonide	19120211	2
Phönix	Triamcinolone acetonide	20000461003	1
Phönix	Triamcinolone acetonide	20002630001	1
Phönix	Triamcinolone acetonide	20002630005	2
Phönix	Triamcinolone acetonide	2001017-01	1
Phönix	Triamcinolone acetonide	2006002-01	2
Phönix	Triamcinolone acetonide	200850209	2
Phönix	Triamcinolone acetonide	2012006-01	2
PHÖNIX	Triamcinolone acetonide	21000116008	1
Phönix	Triamcinolone acetonide	21000116011	1
Phönix	Triamcinolone acetonide	22000902010	1
Phönix	Triamcinolone acetonide	2208004-01	1
Phönix	Triamcinolone acetonide	TAC7	1
Röntgen	Triamcinolone acetonide	1903015-01	1
Sanacorp	Triamcinolone acetonide		1
Sanacorp	Triamcinolone acetonide	100/AKD4	1
Sanacorp	Triamcinolone acetonide	12301506	1
Sanacorp	Triamcinolone acetonide	13124807	2
Sanacorp	Triamcinolone acetonide	1326N11	1
Sanacorp	Triamcinolone acetonide	13379905	1
Sanacorp	Triamcinolone acetonide	13E15-N03	1
sanacorp	Triamcinolone acetonide	15233902	1
Sanacorp	Triamcinolone acetonide	15430108	1
Sanacorp	Triamcinolone acetonide	1710002-01	1
Sanacorp	Triamcinolone acetonide	17120605	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Triamcinolone acetonide	17120610	1
Sanacorp	Triamcinolone acetonide	17358302	1
Sanacorp	Triamcinolone acetonide	17358305	1
Sanacorp	Triamcinolone acetonide	17H03-B12-345553	1
Sanacorp	Triamcinolone acetonide	18100220	1
Sanacorp	Triamcinolone acetonide	18100221	3
Sanacorp	Triamcinolone acetonide	18fB01355724	1
Sanacorp	Triamcinolone acetonide	18K16-B05-359867	1
Sanacorp	Triamcinolone acetonide	191202005	1
Sanacorp	Triamcinolone acetonide	19120208	3
Sanacorp	Triamcinolone acetonide	19120209	1
Sanacorp	Triamcinolone acetonide	2006002-01	1
Sanacorp	Triamcinolone acetonide	20B28-F04-371546	1
Sanacorp	Triamcinolone acetonide	20L18-F01-376658	1
Sanacorp	Triamcinolone acetonide	210001604	1
Sanacorp	Triamcinolone acetonide	2100309093004	1
Sanacorp	Triamcinolone acetonide	2109004-02	1
Sanacorp	Triamcinolone acetonide	21H25-F03-379874	1
Sanacorp	Triamcinolone acetonide	22000902002	1
Sanacorp	Triamcinolone acetonide	2208004-01	1
Sanacorp	Triamcinolone acetonide	2208004-02	1
Sanacorp	Triamcinolone acetonide	22A22-B01-218005	1
Sanacorp	Triamcinolone acetonide	22D15-B01-222391	1
Sanacorp	Triamcinolone acetonide	2308018-01	1
Sanacorp	Triamcinolone acetonide	NY0485M	2
Schulzendorfer Apotheke	Triamcinolone acetonide	2208004-02	1
Sittig	Triamcinolone acetonide	1508008-02	1
Spangro 15.1.2014	Triamcinolone acetonide	1303001-02	1
Spangro 27.03.18	Triamcinolone acetonide	17030337-01	1
Spangropharm	Triamcinolone acetonide	1209040-02	1
Tiarnyao/Gehe	Triamcinolone acetonide	2001017-01	1
VDL	Triamcinolone acetonide	13379903	1
WE: 08.12.2015	Triamcinolone acetonide	14K14-B05-302887	1

- 230 508 spectra from 1515 *Apo-Ident* customers from a total of 48 428 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Triamcinolone acetonide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Triamcinolone acetonide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	722	0	152 240
Type B	0	1679	0	200 405
Type C	0	5501	58	230 508

The substance/substance group *Triamcinolone acetonide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1690 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.6426 %)
Type C	100.0000 % (> 99.9007 %)	98.9566 % (> 98.9027 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20765	20765	0.00	80.12
20910	21061	4.05	79.40
21061	21061	0.00	77.19
21072	21061	4.09	79.24
21587	21587	0.00	79.55
21883	21883	0.00	76.70
21962	21587	14.35	80.92
22313	22313	0.00	76.44
22572	22572	0.00	80.51
22752	22752	0.00	74.14
25339	25339	0.00	159.24
25560	25560	0.00	78.33

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Triclosan**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20005-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Triclosan; Triclosanum

Special notes

When selecting the *Triclosan* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Triclosan	8	17	695

Second-stage model

For differentiation of the substance/substance group *Triclosan* the following second-stage model is used:

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Triclosan* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Oxytetracycline hydrochloride	104.95	–
⋮	⋮	⋮
Sodium citrate	>50	211.15
Capsaicin	>50	284.44
Methoxsalen	>50	328.57
Quinine hydrochloride dihydrate	>50	409.51
Levocarnitine	>50	425.49
Heparin sodium	>50	451.76
Oxybutynin hydrochloride	>50	462.70
Prednicarbate	>50	563.12
Pyridoxal-5-phosphate	>50	568.52
Ciprofloxacin hydrochloride	>50	668.27
Tetracaine	>50	837.62
Alfatradiol	>50	842.79
Cyproterone acetate	>50	950.56
Amifampridine	>50	977.62
Sucrose	>50	1015.40
Norethisterone acetate	>50	1731.38
Amitriptyline hydrochloride	>50	2031.07
Valine	>50	2840.26

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Triclosan* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Triclosan*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Triclosan	13391808	21509	60	20131211
Caelo	Triclosan	14121209	21591	45	20140718

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Triclosan	1406032-01	21615	60	20140710
Euro OTC	Triclosan	1507041	21856	60	20150804*
Euro OTC	Triclosan	1510045	22227	60	20150511*
Euro OTC	Triclosan	1602003	22373	45	20160204*
Euro OTC	Triclosan	1701032	22987	40	20170207*
Fagron	Triclosan	17K02-B06-343548	23915	40	20180105

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 410 spectra of 8 reference samples from the substance/substance group *Triclosan*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 552 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 760 spectra of 20 reference samples from the substance/substance group *Triclosan*.

- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Triclosan	160846	22453	60
Caelo	Triclosan	162808	22775	40
Caelo	Triclosan	171498	23315	40
Caelo	Triclosan	180814	24048	40
Caelo	Triclosan	182537	24387	40
Caelo	Triclosan	192709	25221	40
Caelo	Triclosan	23002009	27331	40
Euro OTC	Triclosan	1607002	22674	40

continued on the next page

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Triclosan	1705011	23425	40
Euro OTC	Triclosan	1708025	23699	40
Euro OTC	Triclosan	1801049	23964	40
Euro OTC	Triclosan	1901006	24466	40
Euro OTC	Triclosan	1912002	24927	40
Euro OTC	Triclosan	2001027	25097	40
Euro OTC	Triclosan	2101029	25578	40
Euro OTC	Triclosan	2206016	26217	40
Fagron	Triclosan	21B25-B02-203360	26284	40
Caelo	Triclosan	23002009	27331SI	20
Euro OTC	Triclosan	2206016	26217SI	20
Fagron	Triclosan	21B25-B02-203360	26284SI	20

- 201 324 spectra from a total of 4028 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6465 spectra from 1263 *Apo-Ident* customers from 732 batches from the substance/substance group *Triclosan*.

- Among them are spectra of independent samples from 676 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Triclosan		1
	Triclosan	/20/11/6107	1
	Triclosan	20J30-B03-204649	1
	Triclosan	21000427001	2
	Triclosan	21000427002	2
	Triclosan	21000427003	3
	Triclosan	21000427005	4
	Triclosan	21000427006	4
	Triclosan	21000427007	1
	Triclosan	21000427008	4
	Triclosan	21000427009	3
	Triclosan	21000427010	1
	Triclosan	21000427011	14
	Triclosan	21000427014	14
	Triclosan	21000427015	8
	Triclosan	21000427016	3
	Triclosan	21000427017	7
	Triclosan	21000428015	1
	Triclosan	21000428016	1
	Triclosan	21000428017	3
	Triclosan	21000428020	9
	Triclosan	21000428021	3
	Triclosan	21000428022	7
	Triclosan	2100427011	1
	Triclosan	2101029-02	2
	Triclosan	2101029-04	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Triclosan	21B25-B02-203359	1
	Triclosan	21B25-B02-203363	1
	Triclosan	21B25-B02-203393	1
	Triclosan	220601601	1
	Triclosan	2206016-01	15
	Triclosan	220601602	1
	Triclosan	2206016-02	9
	Triclosan	2206016-03	2
	Triclosan	2208016-02	1
	Triclosan	23002009001	8
	Triclosan	23002009003	2
18253716	Triclosan		1
30.01.2019 Phoenix	Triclosan	18081415	1
73681 Indien / Gehe	Triclosan	1912002-01	1
73681 Indien / Gehe	Triclosan	1912002-03	1
A.H.D.	Triclosan	12L06-N01	1
AEP	Triclosan	18253722	1
agron/ Noweda	Triclosan	13A11-N03	1
AHC 02.09.13 EK9,04	Triclosan	13D02-N02	1
AHD 17.01.15	Triclosan	13L18-B35-289992	1
AHD	Triclosan	17081723	1
AHD	Triclosan	18081417	2
AHD	Triclosan	18253705	1
AHD	Triclosan	21000427006	1
AHD	Triclosan	21000427007	1
AHD	Triclosan	21000427008	1
AHD	Triclosan	21000427009	2
AHD	Triclosan	21000427017	1
AHD	Triclosan	21000428021	1
AHL	Triclosan	1801049-01	2
ALH	Triclosan	1607002-01	2
Alliance Health 26.1...	Triclosan	13L18-B35-289995	1
Alliance Healthcare/...	Triclosan	13H09-N01	1
Alliance Healthcare	Triclosan	12G09-N09	1
Alliance Healthcare	Triclosan	12L06-N01	1
Alliance Healthcare	Triclosan	13D02-N02	1
Alliance Healthcare	Triclosan	13L-18-835	1
Alliance Healthcare	Triclosan	16084608	1
Alliance/EuRho	Triclosan	1912002-03	3
Alliance	Triclosan	1912002-003	1
Alliance	Triclosan	192709018	1
Alliance	Triclosan	21000427008	1
Alliance	Triclosan	21000427011	1
Alliance	Triclosan	21000428005	1
alliance	Triclosan	21000428022	2
Alliance	Triclosan	2101029-02	1
Alliance	Triclosan	23002009003	2
Allianz	Triclosan	1801049-01	1
anzag 20.11.2013	Triclosan	12359114	1
Anzag 4.12.12 ek:8,89	Triclosan	12G17-N04	1
Anzag	Triclosan	12G09-N09	2
Anzag	Triclosan	12G17-N04	3
Anzag	Triclosan	13L18-B35-289995	1
Anzag	Triclosan	1607002-01	2
Anzag	Triclosan	1701032-02	1
Anzag	Triclosan	192709015	1
Anzag	Triclosan	192709022	1
Anzag	Triclosan	2100427015	1
Anzag	Triclosan	5846205	1
Anzag06.	Triclosan	14F23-B02-295758	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
apo-ident	Triclosan	1708025-01	1
apomix	Triclosan	1406032-01	2
apomix	Triclosan	14F23-B02-295760	1
apomix	Triclosan	17149813	1
Apotheke an der Born...	Triclosan	16280817	3
Audor Pharma	Triclosan		2
BASF Chem trade GmbH...	Triclosan	5846205	1
BASF Grenzach GmbH/Phönix	Triclosan	10006226	1
BASF Grenzach GmbH/Phönix	Triclosan	13A11-N03	1
BASF Grenzach GmbH/Phönix	Triclosan	13A11-No3	1
BASF Grenzach GmbH/Phönix	Triclosan	13D02-N02	1
BASF Grenzach GmbH/Phönix	Triclosan	13H09-N01	1
BASF Grenzach/Noweda	Triclosan	5900346	1
BASF	Triclosan	1505009-01	1
BASF	Triclosan	1708025-01	1
Beiersdorf	Triclosan	14F23-B02-295764	1
Bionorica/Phönix	Triclosan	1708025-01	1
Bombastus	Triclosan	12359111	1
Bombastus	Triclosan	12L06-N01	2
Bombastus	Triclosan	13L18-35-289984	1
Bombastus	Triclosan	1408024-01	1
Bombastus	Triclosan	14f23-b02-300219	1
Bombastus	Triclosan	17081726	1
Bombastus	Triclosan	17149809	1
Cael	Triclosan	182537002	1
Caeleo/ Kehr	Triclosan	192709025	1
Caelo	Triclosan		5
Caelo	Triclosan	10206240	1
Caelo	Triclosan	108144416	1
Caelo	Triclosan	11076716	1
Caelo	Triclosan	11076717	2
Caelo	Triclosan	11238003	2
Caelo	Triclosan	11238004	1
Caelo	Triclosan	11238009	2
Caelo	Triclosan	11238011	1
Caelo	Triclosan	1125204	1
Caelo	Triclosan	1149806	1
Caelo	Triclosan	11777748	3
Caelo	Triclosan	12003201	3
Caelo	Triclosan	12003202	1
Caelo	Triclosan	12003205	7
Caelo	Triclosan	12003210	5
Caelo	Triclosan	12145901	5
Caelo	Triclosan	12145902	5
Caelo	Triclosan	12145906	6
Caelo	Triclosan	12145907	9
Caelo	Triclosan	12145908	7
Caelo	Triclosan	12145909	11
Caelo	Triclosan	12145910	11
Caelo	Triclosan	12145917	1
Caelo	Triclosan	12276827	1
Caelo	Triclosan	12359104	6
Caelo	Triclosan	12359105	7
Caelo	Triclosan	12359106	11
Caelo	Triclosan	12359107	1
Caelo	Triclosan	12359108	13
Caelo	Triclosan	12359109	3
Caelo	Triclosan	12359110	5
Caelo	Triclosan	12359111	7
Caelo	Triclosan	12359112	8

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triclosan	12359114	1
Caelo	Triclosan	12537002	1
Caelo	Triclosan	12680801	1
Caelo	Triclosan	1280801	1
Caelo	Triclosan	12c21-n05	1
Caelo	Triclosan	12G17-N04	2
Caelo	Triclosan	12106-n01	1
Caelo	Triclosan	12L06-N01	7
Caelo	Triclosan	12L06-N01/0005900346	1
Caelo	Triclosan	13247805	1
Caelo	Triclosan	13247903	1
Caelo	Triclosan	13247904	11
Caelo	Triclosan	13247905	10
Caelo	Triclosan	13247908	2
Caelo	Triclosan	13391801	2
Caelo	Triclosan	13391802	4
Caelo	Triclosan	13391804	10
Caelo	Triclosan	13391807	3
Caelo	Triclosan	13391808	9
Caelo	Triclosan	13A11-N03	2
Caelo	Triclosan	13D02-N02	7
Caelo	Triclosan	13D02-No2	1
Caelo	Triclosan	13H08-N10	2
Caelo	Triclosan	13H09-N01	7
Caelo	Triclosan	13L18-B35-289984	1
Caelo	Triclosan	13L18B35289986	1
Caelo	Triclosan	13L18-B35-289986	2
Caelo	Triclosan	13L18-B35-289987	1
Caelo	Triclosan	13L18-B35-289992	2
Caelo	Triclosan	13L18B35289993	1
Caelo	Triclosan	13L18-B35-289995	1
Caelo	Triclosan	14052101	5
Caelo	Triclosan	14052102	11
Caelo	Triclosan	14052103	14
Caelo	Triclosan	14052105	1
Caelo	Triclosan	1412109	1
Caelo	Triclosan	14121203	10
Caelo	Triclosan	14121204	9
Caelo	Triclosan	14121207	10
Caelo	Triclosan	14121209	6
Caelo	Triclosan	14121210	11
Caelo	Triclosan	14121211	9
Caelo	Triclosan	14121214	13
Caelo	Triclosan	14121215	14
Caelo	Triclosan	14121220	1
Caelo	Triclosan	1418E-03402	1
Caelo	Triclosan	14205901	7
Caelo	Triclosan	14205902	9
Caelo	Triclosan	14205903	15
Caelo	Triclosan	14205904	6
Caelo	Triclosan	14205905	6
Caelo	Triclosan	14211207	1
Caelo	Triclosan	14211211	1
Caelo	Triclosan	14F23-B02	1
Caelo	Triclosan	14F23B02293859	1
Caelo	Triclosan	14F23-B02-295758	1
Caelo	Triclosan	14F23-B02-295760	1
Caelo	Triclosan	14F23-B02-295765	1
Caelo	Triclosan	150103201	1
Caelo	Triclosan	1501032-02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triclosan	1503603	1
Caelo	Triclosan	1505009	1
Caelo	Triclosan	150704101	1
Caelo	Triclosan	1507041-01	2
Caelo	Triclosan	15121202	1
Caelo	Triclosan	15203603	14
Caelo	Triclosan	15203604	14
Caelo	Triclosan	15203606	9
Caelo	Triclosan	15203607	15
Caelo	Triclosan	15203608	11
Caelo	Triclosan	1520603	1
Caelo	Triclosan	1530105	1
Caelo	Triclosan	15301501	1
Caelo	Triclosan	15301502	13
Caelo	Triclosan	15301503	12
Caelo	Triclosan	15301504	12
Caelo	Triclosan	15301505	12
Caelo	Triclosan	15301506	18
Caelo	Triclosan	15301510	2
Caelo	Triclosan	15301511	9
Caelo	Triclosan	15301512	6
Caelo	Triclosan	15301513	1
Caelo	Triclosan	15301514	1
Caelo	Triclosan	15c10-b06	1
Caelo	Triclosan	15C10-B06-310031	3
Caelo	Triclosan	15C10-B06-310031	1
Caelo	Triclosan	15C10-B06-311161	1
Caelo	Triclosan	15C10-B06-312982	3
Caelo	Triclosan	15G07-B03-30039	1
Caelo	Triclosan	15G07-B03-310035	1
Caelo	Triclosan	15G07-B03-310035/201	1
Caelo	Triclosan	15G07-B03-310037	2
Caelo	Triclosan	15G07-B03-310038	2
Caelo	Triclosan	15G07-B03-310040	1
Caelo	Triclosan	160084601	1
Caelo	Triclosan	1602003-01	2
Caelo	Triclosan	16021306	1
Caelo	Triclosan	160280811	1
Caelo	Triclosan	16064616	1
Caelo	Triclosan	1607002-01	2
Caelo	Triclosan	16071801	1
Caelo	Triclosan	160846	1
Caelo	Triclosan	16084601	7
Caelo	Triclosan	160846018	1
Caelo	Triclosan	16084602	10
Caelo	Triclosan	16084603	15
Caelo	Triclosan	16084606	5
Caelo	Triclosan	16084607	11
Caelo	Triclosan	16084608	17
Caelo	Triclosan	16084609	3
Caelo	Triclosan	16084610	11
Caelo	Triclosan	16084611	17
Caelo	Triclosan	16084614	20
Caelo	Triclosan	16084617	1
Caelo	Triclosan	16084618	16
Caelo	Triclosan	16084620	1
Caelo	Triclosan	16084621	1
Caelo	Triclosan	16084622	1
Caelo	Triclosan	1609005	1
Caelo	Triclosan	1609005-02	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triclosan	1620809	1
Caelo	Triclosan	16253716	1
Caelo	Triclosan	162808	1
Caelo	Triclosan	16280801	29
Caelo	Triclosan	16280802	23
Caelo	Triclosan	16280802-30417/1	1
Caelo	Triclosan	16280803	5
Caelo	Triclosan	16280805	2
Caelo	Triclosan	16280808	21
Caelo	Triclosan	16280809	8
Caelo	Triclosan	16280810	1
Caelo	Triclosan	16280811	19
Caelo	Triclosan	16280816	17
Caelo	Triclosan	16280817	14
Caelo	Triclosan	16280818	7
Caelo	Triclosan	16280819	7
Caelo	Triclosan	1628082	1
Caelo	Triclosan	16280820	13
Caelo	Triclosan	16280821	2
Caelo	Triclosan	16280824	4
Caelo	Triclosan	16280874	1
Caelo	Triclosan	162820817	1
Caelo	Triclosan	16293901	1
Caelo	Triclosan	1701032	1
Caelo	Triclosan	1701032-01	3
Caelo	Triclosan	170501101	2
Caelo	Triclosan	1705011-01	7
Caelo	Triclosan	170802-01	1
Caelo	Triclosan	170802501	1
Caelo	Triclosan	1708025-01	4
Caelo	Triclosan	170817	1
Caelo	Triclosan	17081702	1
Caelo	Triclosan	17081703	11
Caelo	Triclosan	17081704	1
Caelo	Triclosan	17081705	12
Caelo	Triclosan	17081706	4
Caelo	Triclosan	17081707	26
Caelo	Triclosan	170817075274	1
Caelo	Triclosan	17081709	20
Caelo	Triclosan	17081710	19
Caelo	Triclosan	17081711	17
Caelo	Triclosan	17081712	18
Caelo	Triclosan	17081713	9
Caelo	Triclosan	17081714	12
Caelo	Triclosan	17081716	17
Caelo	Triclosan	17081716-T20180112Ma	1
Caelo	Triclosan	17081717	8
Caelo	Triclosan	17081720	31
Caelo	Triclosan	17081721	24
Caelo	Triclosan	17081722	30
Caelo	Triclosan	17081723	10
Caelo	Triclosan	17081724	23
Caelo	Triclosan	17081725	19
Caelo	Triclosan	17081726	16
Caelo	Triclosan	170817265507	1
Caelo	Triclosan	1708173	1
Caelo	Triclosan	170919Di	1
Caelo	Triclosan	171449809	1
Caelo	Triclosan	1714819	1
Caelo	Triclosan	17148927	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triclosan	1714926	1
Caelo	Triclosan	1714930	1
Caelo	Triclosan	17149621	1
Caelo	Triclosan	171498	1
Caelo	Triclosan	17149801	5
Caelo	Triclosan	17149805	10
Caelo	Triclosan	17149806	13
Caelo	Triclosan	17149807	17
Caelo	Triclosan	17149808	40
Caelo	Triclosan	171498085598	1
Caelo	Triclosan	17149809	50
Caelo	Triclosan	17149810P-190531-3	1
Caelo	Triclosan	17149812	16
Caelo	Triclosan	17149812-20180619Ma4	1
Caelo	Triclosan	17149813	19
Caelo	Triclosan	17149813-T20181115Ma	1
Caelo	Triclosan	17149814	20
Caelo	Triclosan	17149815	14
Caelo	Triclosan	17149817	6
Caelo	Triclosan	17149818	1
Caelo	Triclosan	17149819	32
Caelo	Triclosan	17149820	20
Caelo	Triclosan	17149821	39
Caelo	Triclosan	17149822	15
Caelo	Triclosan	17149824	9
Caelo	Triclosan	17149825	26
Caelo	Triclosan	17149826	1
Caelo	Triclosan	17149827	22
Caelo	Triclosan	171499808	1
Caelo	Triclosan	171499815	1
Caelo	Triclosan	171549805	1
Caelo	Triclosan	1719809	1
Caelo	Triclosan	1719814	1
Caelo	Triclosan	1748912	1
Caelo	Triclosan	1749825	1
Caelo	Triclosan	17801712	1
Caelo	Triclosan	1781720	1
Caelo	Triclosan	17K02-B06_343544	2
Caelo	Triclosan	17K02-B06-343543	1
Caelo	Triclosan	180081408	1
Caelo	Triclosan	1801417	1
Caelo	Triclosan	18061407	1
Caelo	Triclosan	180811401	1
Caelo	Triclosan	18081401	8
Caelo	Triclosan	18081402	21
Caelo	Triclosan	18081403	15
Caelo	Triclosan	18081405	43
Caelo	Triclosan	18081406	33
Caelo	Triclosan	18081407	37
Caelo	Triclosan	18081408	55
Caelo	Triclosan	18081409	1
Caelo	Triclosan	18081410	14
Caelo	Triclosan	18081411	1
Caelo	Triclosan	18081413	39
Caelo	Triclosan	18081414	30
Caelo	Triclosan	18081415	42
Caelo	Triclosan	18081416	37
Caelo	Triclosan	18081417	50
Caelo	Triclosan	1808414	1
Caelo	Triclosan	18243726	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triclosan	18253/06	1
Caelo	Triclosan	18253078	1
Caelo	Triclosan	182533722	1
Caelo	Triclosan	182537001	61
Caelo	Triclosan	182537002	51
Caelo	Triclosan	18253701	6
Caelo	Triclosan	18253702	12
Caelo	Triclosan	18253703	3
Caelo	Triclosan	18253705	47
Caelo	Triclosan	182537052	1
Caelo	Triclosan	18253706	41
Caelo	Triclosan	18253707	38
Caelo	Triclosan	18253708	42
Caelo	Triclosan	18253709	32
Caelo	Triclosan	18253710	8
Caelo	Triclosan	18253711	33
Caelo	Triclosan	18253712	28
Caelo	Triclosan	18253713P-200116-1	1
Caelo	Triclosan	18253714	11
Caelo	Triclosan	18253715	3
Caelo	Triclosan	18253716	57
Caelo	Triclosan	18253717	19
Caelo	Triclosan	18253718	22
Caelo	Triclosan	18253721	30
Caelo	Triclosan	18253722	35
Caelo	Triclosan	18253724	6
Caelo	Triclosan	182537247	1
Caelo	Triclosan	18253726	17
Caelo	Triclosan	18253729	1
Caelo	Triclosan	18253731	2
Caelo	Triclosan	1825717	1
Caelo	Triclosan	182597001	1
Caelo	Triclosan	185237002	1
Caelo	Triclosan	18523716	1
Caelo	Triclosan	1852537001	1
Caelo	Triclosan	185253711	1
Caelo	Triclosan	1901006-01	1
Caelo	Triclosan	1901006-02	1
Caelo	Triclosan	1901006-03	1
Caelo	Triclosan	190709021	1
Caelo	Triclosan	1912002-01	1
Caelo	Triclosan	1912002-03	3
Caelo	Triclosan	192109015	1
Caelo	Triclosan	1922709021	1
Caelo	Triclosan	1927009013	1
Caelo	Triclosan	192708022	1
Caelo	Triclosan	192709002	24
Caelo	Triclosan	192709003	10
Caelo	Triclosan	192709004	18
Caelo	Triclosan	192709006	1
Caelo	Triclosan	192709007	11
Caelo	Triclosan	192709008	1
Caelo	Triclosan	192709009	8
Caelo	Triclosan	192709010	16
Caelo	Triclosan	192709011	30
Caelo	Triclosan	192709012	34
Caelo	Triclosan	192709013	20
Caelo	Triclosan	192709014	34
Caelo	Triclosan	192709014/4720	1
Caelo	Triclosan	192709015	31

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triclosan	192709016	32
Caelo	Triclosan	192709018	8
Caelo	Triclosan	192709020	41
Caelo	Triclosan	192709021	49
Caelo	Triclosan	192709022	32
Caelo	Triclosan	192709023	14
Caelo	Triclosan	192709025	31
Caelo	Triclosan	19270913	1
Caelo	Triclosan	1927099021	1
Caelo	Triclosan	19709007	1
Caelo	Triclosan	2000428001	1
Caelo	Triclosan	20021304	1
Caelo	Triclosan	200701407	1
Caelo	Triclosan	200870409	1
Caelo	Triclosan	21000427	1
Caelo	Triclosan	21000427001	13
Caelo	Triclosan	21000427002	6
Caelo	Triclosan	21000427005	4
Caelo	Triclosan	21000427006	2
Caelo	Triclosan	21000427007	11
Caelo	Triclosan	21000427008	1
Caelo	Triclosan	21000427009	1
Caelo	Triclosan	21000427011	3
Caelo	Triclosan	21000427017	1
Caelo	Triclosan	21000428001	33
Caelo	Triclosan	21000428002	1
Caelo	Triclosan	21000428003	23
Caelo	Triclosan	21000428004	21
Caelo	Triclosan	21000428005	7
Caelo	Triclosan	21000428008	24
Caelo	Triclosan	21000428009	23
Caelo	Triclosan	2100042801	1
Caelo	Triclosan	21000428010	21
Caelo	Triclosan	21000428011	17
Caelo	Triclosan	21000428012	13
Caelo	Triclosan	21000428013	7
Caelo	Triclosan	21000428015	16
Caelo	Triclosan	21000428016	16
Caelo	Triclosan	21000428017	10
Caelo	Triclosan	21000428021	11
Caelo	Triclosan	2100042812	1
Caelo	Triclosan	21000828001	1
Caelo	Triclosan	2100427001	1
Caelo	Triclosan	2100428001	4
Caelo	Triclosan	2100428011	1
Caelo	Triclosan	228711-514	1
Caelo	Triclosan	23121409	1
Caelo	Triclosan	2317I-03402	1
Caelo	Triclosan	28011	1
Caelo	Triclosan	3041408	1
Caelo	Triclosan	39(192709020)	1
Caelo	Triclosan	5012E-03402	1
Caelo	Triclosan	517E-03402	1
Caelo	Triclosan	5203607	1
Caelo	Triclosan	6121711	1
Caelo	Triclosan	8081401	1
Caelo	Triclosan	8253718	1
Caelo	Triclosan	87767	1
Caelo	Triclosan	AKD12	1
Caelo	Triclosan	bhfdd	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Triclosan	Caelo	2
Caeo/Noweda	Triclosan	15301505	1
Caeo/Sanacorp	Triclosan	18081405	1
Caeolo/Noweda	Triclosan	13247905	1
Caeolo/Phönix	Triclosan	18081416	1
Caeolo	Triclosan	17149809	1
Caesar & Lorenz GmbH	Triclosan	192709016	1
Caesar & Lorenz	Triclosan	21000428020	1
Caesar & Loretz GmbH…	Triclosan	18253721	1
Caesar & Loretz GmbH…	Triclosan	21000428015	1
Caesar & Loretz GmbH…	Triclosan	182537001	1
Caesar & Loretz GmbH…	Triclosan	18253708	1
Caesar & Loretz GmbH…	Triclosan	18253717	1
Caesar & Loretz GmbH…	Triclosan	21000427011	2
Caesar & Loretz GmbH…	Triclosan	192709015	2
Caesar & Loretz GmbH…	Triclosan	192709016	2
Caesar & Loretz GmbH…	Triclosan	17149813	1
Caesar & Loretz GmbH…	Triclosan	18081413	2
Caesar & Loretz GmbH…	Triclosan	18081416	1
Caesar & Loretz GmbH…	Triclosan	21000427001	2
Caesar & Loretz GmbH…	Triclosan	18253705	1
Caesar & Loretz GmbH…	Triclosan	18253730	1
Caesar & Loretz GmbH…	Triclosan	18081417	1
Caesar & Loretz GmbH…	Triclosan	18253709	2
Caesar & Loretz GmbH…	Triclosan	18253710	1
Caesar & Loretz GmbH…	Triclosan	18253707	1
Caesar & Loretz GmbH/ AHD	Triclosan	18081416	1
Caesar & Loretz GmbH…	Triclosan	192709016	2
Caesar & Loretz GmbH…	Triclosan	21000428008	1
Caesar & Loretz GmbH…	Triclosan	192709022	2
Caesar & Loretz GmbH…	Triclosan	192709020	2
Caesar & Loretz GmbH…	Triclosan	21000427003	1
Caesar & Loretz GmbH…	Triclosan	192709022	1
Caesar & Loretz GmbH/AHD	Triclosan	192709011	1
Caesar & Loretz GmbH/AHD	Triclosan	21000428021	2
Caesar & Loretz GmbH…	Triclosan	192709020	2
Caesar & Loretz GmbH…	Triclosan	18081408	1
Caesar & Loretz GmbH…	Triclosan	18081417	1
Caesar & Loretz GmbH…	Triclosan	192709016	1
Caesar & Loretz GmbH…	Triclosan	192709021	1
Caesar & Loretz GmbH…	Triclosan	21000428011	1
Caesar & Loretz GmbH/Gehe	Triclosan	18253708	1
Caesar & Loretz GmbH/Gehe	Triclosan	192709012	1
Caesar & Loretz GmbH/Gehe	Triclosan	192709013	1
Caesar & Loretz GmbH/Gehe	Triclosan	192709014	1
Caesar & Loretz GmbH/Gehe	Triclosan	192709016	1
Caesar & Loretz GmbH/Gehe	Triclosan	192709025	1
Caesar & Loretz GmbH/Gehe	Triclosan	21000427002	1
Caesar & Loretz GmbH/Gehe	Triclosan	21000428010	1
Caesar & Loretz GmbH/Gehe	Triclosan	21000428011	2
Caesar & Loretz GmbH…	Triclosan	18253707	1
Caesar & Loretz GmbH…	Triclosan	192709002	1
Caesar & Loretz GmbH…	Triclosan	192709009	1
Caesar & Loretz GmbH…	Triclosan	192709012	1
Caesar & Loretz GmbH…	Triclosan	192709022	1
Caesar & Loretz GmbH…	Triclosan	21000428001	1
Caesar & Loretz GmbH…	Triclosan	21000428009	1
Caesar & Loretz GmbH…	Triclosan	21000428010	1
Caesar & Loretz GmbH…	Triclosan	21000428011	1
Caesar & Loretz GmbH…	Triclosan	AP210406-01	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Kehr	Triclosan	18253707	1
Caesar & Loretz GmbH/Kehr	Triclosan	18253712	1
Caesar & Loretz GmbH/Kehr	Triclosan	18253721	1
Caesar & Loretz GmbH/Kehr	Triclosan	192709014	1
Caesar & Loretz GmbH/Kehr	Triclosan	21000427002	1
Caesar & Loretz GmbH/Kehr	Triclosan	21000428003	1
Caesar & Loretz GmbH...	Triclosan	18081413	1
Caesar & Loretz GmbH...	Triclosan	18253721	1
Caesar & Loretz GmbH...	Triclosan	18253708	1
Caesar & Loretz GmbH...	Triclosan	18081407	1
Caesar & Loretz GmbH...	Triclosan	182537002	1
Caesar & Loretz GmbH...	Triclosan	18253711	3
Caesar & Loretz GmbH...	Triclosan	192709003	1
Caesar & Loretz GmbH...	Triclosan	192709007	2
Caesar & Loretz GmbH...	Triclosan	192709018	4
Caesar & Loretz GmbH...	Triclosan	192709020	2
Caesar & Loretz GmbH...	Triclosan	21000428004	1
Caesar & Loretz GmbH...	Triclosan	21000428015	2
Caesar & Loretz GmbH...	Triclosan	21000428017	1
Caesar & Loretz GmbH...	Triclosan	21000427007	2
Caesar & Loretz GmbH...	Triclosan	21000428003	1
Caesar & Loretz GmbH...	Triclosan	21000428010	1
Caesar & Loretz GmbH...	Triclosan	21000428011	2
Caesar & Loretz GmbH...	Triclosan	18253718	4
Caesar & Loretz GmbH...	Triclosan	18253712	1
Caesar & Loretz GmbH...	Triclosan	182537002	4
Caesar & Loretz GmbH...	Triclosan	18253706	1
Caesar & Loretz GmbH...	Triclosan	18253714	1
Caesar & Loretz GmbH...	Triclosan	18253722	1
Caesar & Loretz GmbH...	Triclosan	192709016	1
Caesar & Loretz GmbH...	Triclosan	192709021	1
Caesar & Loretz GmbH...	Triclosan	192709025	2
Caesar & Loretz GmbH...	Triclosan	21000427001	1
Caesar & Loretz GmbH...	Triclosan	21000428001	2
Caesar & Loretz GmbH...	Triclosan	21000428003	1
Caesar & Loretz GmbH...	Triclosan	21000428005	1
Caesar & Loretz GmbH...	Triclosan	21000428011	1
Caesar & Loretz GmbH...	Triclosan	18253711	1
Caesar & Loretz GmbH...	Triclosan	18253721	2
Caesar & Loretz GmbH...	Triclosan	18253722	1
Caesar & Loretz GmbH...	Triclosan	192709011	1
Caesar & Loretz GmbH...	Triclosan	192709013	2
Caesar & Loretz GmbH...	Triclosan	192709021	1
Caesar & Loretz GmbH...	Triclosan	192709021	1
Caesar & Loretz GmbH...	Triclosan	21000428009	3
Caesar & Loretz GmbH...	Triclosan	21000428012	2
Caesar & Loretz GmbH...	Triclosan	21000428015	1
Caesar & Loretz GmbH...	Triclosan	21000428017	1
Caesar & Loretz GmbH	Triclosan	15081416	1
Caesar & Loretz GmbH	Triclosan	1609005-01	1
Caesar & Loretz GmbH	Triclosan	16280811	1
Caesar & Loretz GmbH	Triclosan	17149806	1
Caesar & Loretz GmbH	Triclosan	17149813	1
Caesar & Loretz GmbH	Triclosan	17149821	1
Caesar & Loretz GmbH	Triclosan	18081403	1
Caesar & Loretz GmbH	Triclosan	18081410	1
Caesar & Loretz GmbH	Triclosan	18081413	1
Caesar & Loretz GmbH	Triclosan	18081414	3
Caesar & Loretz GmbH	Triclosan	18081416	4
Caesar & Loretz GmbH	Triclosan	18081417	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Triclosan	182537001	13
Caesar & Loretz GmbH	Triclosan	182537002	9
Caesar & Loretz GmbH	Triclosan	18253702	2
Caesar & Loretz GmbH	Triclosan	18253705	9
Caesar & Loretz GmbH	Triclosan	18253706	13
Caesar & Loretz GmbH	Triclosan	18253707	5
Caesar & Loretz GmbH	Triclosan	18253708	5
Caesar & Loretz GmbH	Triclosan	18253709	9
Caesar & Loretz GmbH	Triclosan	18253710	6
Caesar & Loretz GmbH	Triclosan	18253711	3
Caesar & Loretz GmbH	Triclosan	18253712	4
Caesar & Loretz GmbH	Triclosan	18253714	2
Caesar & Loretz GmbH	Triclosan	18253716	19
Caesar & Loretz GmbH	Triclosan	18253717	4
Caesar & Loretz GmbH	Triclosan	18253718	7
Caesar & Loretz GmbH	Triclosan	18253721	5
Caesar & Loretz GmbH	Triclosan	18253722	2
Caesar & Loretz GmbH	Triclosan	18253724	2
Caesar & Loretz GmbH	Triclosan	18253726	6
Caesar & Loretz GmbH	Triclosan	190100602	1
Caesar & Loretz GmbH	Triclosan	1912002-01	1
Caesar & Loretz GmbH	Triclosan	1912002-04	1
Caesar & Loretz GmbH	Triclosan	192709002	6
Caesar & Loretz GmbH	Triclosan	192709003	1
Caesar & Loretz GmbH	Triclosan	192709004	3
Caesar & Loretz GmbH	Triclosan	192709009	1
Caesar & Loretz GmbH	Triclosan	192709010	2
Caesar & Loretz GmbH	Triclosan	192709011	7
Caesar & Loretz GmbH	Triclosan	192709012	6
Caesar & Loretz GmbH	Triclosan	192709013	9
Caesar & Loretz GmbH	Triclosan	192709014	5
Caesar & Loretz GmbH	Triclosan	192709015	12
Caesar & Loretz GmbH	Triclosan	192709016	8
Caesar & Loretz GmbH	Triclosan	192709018	5
Caesar & Loretz GmbH	Triclosan	192709020	14
Caesar & Loretz GmbH	Triclosan	192709021	21
Caesar & Loretz GmbH	Triclosan	192709022	13
Caesar & Loretz GmbH	Triclosan	192709023	3
Caesar & Loretz GmbH	Triclosan	192709024	1
Caesar & Loretz GmbH	Triclosan	192709025	5
Caesar & Loretz GmbH	Triclosan	19279003	2
Caesar & Loretz GmbH	Triclosan	20003964012	1
Caesar & Loretz GmbH	Triclosan	2001027-01	1
Caesar & Loretz GmbH	Triclosan	21000427001	7
Caesar & Loretz GmbH	Triclosan	21000427003	2
Caesar & Loretz GmbH	Triclosan	21000427005	1
Caesar & Loretz GmbH	Triclosan	21000427007	4
Caesar & Loretz GmbH	Triclosan	21000427008	1
Caesar & Loretz GmbH	Triclosan	21000427011	2
Caesar & Loretz GmbH	Triclosan	21000428001	9
Caesar & Loretz GmbH	Triclosan	21000428003	8
Caesar & Loretz GmbH	Triclosan	21000428004	4
Caesar & Loretz GmbH	Triclosan	21000428005	1
Caesar & Loretz GmbH	Triclosan	21000428008	8
Caesar & Loretz GmbH	Triclosan	21000428009	6
Caesar & Loretz GmbH	Triclosan	21000428010	7
Caesar & Loretz GmbH	Triclosan	21000428011	13
Caesar & Loretz GmbH	Triclosan	21000428012	7
Caesar & Loretz GmbH	Triclosan	21000428013	4
Caesar & Loretz GmbH	Triclosan	21000428015	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Triclosan	21000428016	4
Caesar & Loretz GmbH	Triclosan	21000428017	4
Caesar & Loretz GmbH	Triclosan	21000428018	1
Caesar & Loretz GmbH	Triclosan	21000428021	4
Caesar & Loretz GmbH	Triclosan	AP210205-02	1
Caesar & Loretz Hild…	Triclosan	192709013	1
Caesar & Loretz Hilden	Triclosan	18081408	1
Caesar & Loretz Hilden	Triclosan	18081413	1
Caesar & Loretz Hilden	Triclosan	18081414	1
Caesar & Loretz Hilden	Triclosan	18081417	2
Caesar & Loretz Hilden	Triclosan	182537001	2
Caesar & Loretz Hilden	Triclosan	18253707	1
Caesar & Loretz Hilden	Triclosan	18253709	1
Caesar & Loretz Hilden	Triclosan	18253710	1
Caesar & Loretz Hilden	Triclosan	18253717	1
Caesar & Loretz Hilden	Triclosan	18253726	1
Caesar & Loretz Hilden	Triclosan	192709002	1
Caesar & Loretz Hilden	Triclosan	192709011	1
Caesar & Loretz/ Noweda	Triclosan	17149812	1
Caesar & Loretz/AHC	Triclosan	16084603	2
Caesar & Loretz/AHD	Triclosan	14121209	1
Caesar & Loretz	Triclosan	17081705	1
Caesar / Ebert	Triclosan	17081716	1
Caesar / Gehe	Triclosan	18253709	1
Caesar u Loretz	Triclosan	15301503	1
Caesar und Loretz GmbH	Triclosan	17149808	1
Caesar und Loretz	Triclosan	15301502	1
Caesar&Lorenz / Gehe	Triclosan	18253716	1
Caesar&Lorenz / Gehe	Triclosan	18253722	1
Caesar&Lorenz	Triclosan	17081707	1
Caesar&Lorenz	Triclosan	21000428001	1
Caesar&Lorenz	Triclosan	21000428010	1
Caesar&Loretz GmbH/Anzag	Triclosan	14121215	2
Caesar&Loretz GmbH/Anzag	Triclosan	15203603	2
Caesar&Loretz GmbH/S…	Triclosan	15301505	1
Caesar&Loretz GmbH	Triclosan	16084609	1
Caesar&Loretz GmbH	Triclosan	16280808	1
Caesar&Loretz GmbH	Triclosan	192709002	1
Caesar&Loretz GmbH	Triclosan	192709025	1
Caesar&Loretz,AHC,12…	Triclosan	16084618	1
Caesar&loretz,Phönix	Triclosan	15203606	1
caesar&loretz,Phönix	Triclosan	15203607	1
Caesar/Lorenz	Triclosan	12145910	1
Caesar/Lorenz	Triclosan	12359104	1
Caesar/Lorenz	Triclosan	13247904	1
Caleo/Phönix	Triclosan	17081711	1
Carlo/Phönix/23,50	Triclosan	1901006-01	1
Cealo/AHD	Triclosan	14F23-B02-295947	1
Cealo/Anzag	Triclosan	182537002	1
Cealo/Gehe	Triclosan	17149807	1
Cealo/Phoenix	Triclosan	192709015	1
Cealo/Sanacorp	Triclosan	192709025	1
Cealo	Triclosan	16280801	1
Cealo	Triclosan	17081723	1
Cealo	Triclosan	17149809	1
Cealo	Triclosan	18081403	1
Cealo	Triclosan	18081405	1
Cealo	Triclosan	18081416	1
Cealo	Triclosan	192709016	1
Cealo	Triclosan	21000428003	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Cealo	Triclosan	71215/1Gie	1
Celo/Phonix	Triclosan	16084611	1
Crystal pharma/ Ober…	Triclosan	15203603	1
DAB 2008	Triclosan	12003201	2
Delta Apotheke	Triclosan	17149822	1
E Plus	Triclosan	16280808	1
E Plus	Triclosan	17081705	1
Easy Höchst	Triclosan	17149822	1
ebe a	Triclosan	14121207	1
Eigenproduktion	Triclosan	13A11-N03	1
EuRho / 30	Triclosan	1401038-01	1
EuRho / fiebig	Triclosan	1705011-01	1
EuRho / Fiebig	Triclosan	2001027	1
EuRho /11	Triclosan	1912002-01	1
EuRho Gehe	Triclosan	1801049-01	1
EuRho GEHE	Triclosan	1912002-01	2
EuRho/ Phoenix	Triclosan	2101029-01	1
Eurho/A	Triclosan	2101029-01	2
eurho/AHC	Triclosan	2001027-01	1
EuRho/Gehe	Triclosan	1912002-02	1
EuRho/Gehe	Triclosan	2001027-01	1
EuRho/Noweda	Triclosan	1708025-01	2
EuRho/Noweda	Triclosan	1901006-03	1
EuRho/Phoenix	Triclosan	1401038-01	1
EuRho/Phönix	Triclosan	1307050-01	2
EuRho/Phönix	Triclosan	1912002-01	1
EuRho/Phönix	Triclosan	1912002-02	1
Eurho/Phönix	Triclosan	210102901	1
Eurho/S	Triclosan	2101029-02	1
Eurho/Sanacorp	Triclosan	2101029-01	1
EuRho	Triclosan	1107030-01	2
EuRho	Triclosan	1202018-01	1
EuRho	Triclosan	1206034-02	2
EuRho	Triclosan	1408024-01	1
EuRho	Triclosan	151004501	1
EuRho	Triclosan	1705011-01	1
EuRho	Triclosan	1708025-01	1
EuRho	Triclosan	1901006-01	1
EuRho	Triclosan	1901006-02	4
EuRho	Triclosan	1901006-03	1
EuRho	Triclosan	1912002-01	1
euRho	Triclosan	191200204	1
EuRho	Triclosan	2101029-01	1
Eurho	Triclosan	2101029-02	1
EuRho	Triclosan	2101029-02	3
EuRho	Triclosan	k0011	1
EuRhoNoweda	Triclosan	1602003-01	1
Euro OCT/Noweda	Triclosan	1501032-02	1
Euro OCT	Triclosan	1912002-01	1
Euro OTC	Triclosan		13
Euro OTC	Triclosan	/19/07/3301	1
Euro OTC	Triclosan	/20/11/6107	2
Euro OTC	Triclosan	1107030-01	3
Euro OTC	Triclosan	1202018-01	1
Euro OTC	Triclosan	1202018-02	2
Euro OTC	Triclosan	120203-02	1
Euro OTC	Triclosan	1206034-01	1
Euro OTC	Triclosan	120603402	1
Euro OTC	Triclosan	1206034-02	3
Euro OTC	Triclosan	1211025-01	11

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Triclosan	12276023	2
Euro OTC	Triclosan	12276024	1
Euro OTC	Triclosan	12276027	3
Euro OTC	Triclosan	12276028	5
Euro OTC	Triclosan	1245	1
Euro OTC	Triclosan	130301101	1
Euro OTC	Triclosan	1303011-01	5
Euro OTC	Triclosan	1307050-01	6
Euro OTC	Triclosan	13247904	1
Euro OTC	Triclosan	13H08-N10	1
Euro OTC	Triclosan	140103801	1
Euro OTC	Triclosan	1401038-01	10
Euro OTC	Triclosan	140603201	1
Euro OTC	Triclosan	1406032-01	10
Euro OTC	Triclosan	1408024-01	6
Euro OTC	Triclosan	14121204	1
Euro OTC	Triclosan	14F23-B02-295948	1
Euro OTC	Triclosan	1501032-01	10
Euro OTC	Triclosan	1501032-02	4
Euro OTC	Triclosan	150500901	1
Euro OTC	Triclosan	1505009-01	12
Euro OTC	Triclosan	15058946	2
Euro OTC	Triclosan	1507041-01	7
Euro OTC	Triclosan	151004501	1
Euro OTC	Triclosan	1510045-01	19
Euro OTC	Triclosan	15150229	2
Euro OTC	Triclosan	15203607	3
Euro OTC	Triclosan	1550229	1
Euro OTC	Triclosan	15C10-B06-312981	1
Euro OTC	Triclosan	15C10-B06-312982	1
Euro OTC	Triclosan	15G07-B03-310036	1
Euro OTC	Triclosan	15G07-B03-310040	1
Euro OTC	Triclosan	1602003	2
Euro OTC	Triclosan	160200301	1
Euro OTC	Triclosan	1602003-01	29
Euro OTC	Triclosan	16047002-01	1
Euro OTC	Triclosan	160531T	1
Euro OTC	Triclosan	160700201	1
Euro OTC	Triclosan	1607002-01	34
Euro OTC	Triclosan	160702-01	1
Euro OTC	Triclosan	16084614	1
Euro OTC	Triclosan	160900-02	1
Euro OTC	Triclosan	16090005-02	1
Euro OTC	Triclosan	1609005-01	30
Euro OTC	Triclosan	160900502	1
Euro OTC	Triclosan	1609005-02	27
Euro OTC	Triclosan	16280820	1
Euro OTC	Triclosan	169005-02	1
Euro OTC	Triclosan	1701032	1
Euro OTC	Triclosan	1701032_01	1
Euro OTC	Triclosan	1701032-01	17
Euro OTC	Triclosan	170103202	1
Euro OTC	Triclosan	1701032-02	16
Euro OTC	Triclosan	1701037-01	1
Euro OTC	Triclosan	170113T1609005-01	1
Euro OTC	Triclosan	170132-01	1
Euro OTC	Triclosan	170501101	2
Euro OTC	Triclosan	1705011-01	50
Euro OTC	Triclosan	170511-01	1
Euro OTC	Triclosan	170511-010012276028	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Triclosan	170526T/1701032-02	1
Euro OTC	Triclosan	17080-01	1
Euro OTC	Triclosan	1708025	1
Euro OTC	Triclosan	1708025_01	1
Euro OTC	Triclosan	170802501	2
Euro OTC	Triclosan	1708025-01	47
Euro OTC	Triclosan	1708025-01P-181001-3	1
Euro OTC	Triclosan	1708025-01P181129-4	1
Euro OTC	Triclosan	17081703	1
Euro OTC	Triclosan	17081722	1
Euro OTC	Triclosan	170825-01	1
Euro OTC	Triclosan	171121T/1705011-01	1
Euro OTC	Triclosan	17149806	1
Euro OTC	Triclosan	17149808	1
Euro OTC	Triclosan	17149812	1
Euro OTC	Triclosan	17149815	1
Euro OTC	Triclosan	17K02-B06-343548	2
Euro OTC	Triclosan	1801049	1
Euro OTC	Triclosan	1801049-01	12
Euro OTC	Triclosan	1801049-21	1
Euro OTC	Triclosan	180149-01	1
Euro OTC	Triclosan	1805001-01	1
Euro OTC	Triclosan	18253706	2
Euro OTC	Triclosan	1901006	1
Euro OTC	Triclosan	1901006-002	1
Euro OTC	Triclosan	190100601	2
Euro OTC	Triclosan	1901006-01	58
Euro OTC	Triclosan	190100602	2
Euro OTC	Triclosan	1901006-02	33
Euro OTC	Triclosan	1901006-03	17
Euro OTC	Triclosan	1901006-1	3
Euro OTC	Triclosan	1901006-1P-190506-2	1
Euro OTC	Triclosan	191006-02	1
Euro OTC	Triclosan	19120002-02	1
Euro OTC	Triclosan	19120003	1
Euro OTC	Triclosan	1912001-01	1
Euro OTC	Triclosan	1912002	3
Euro OTC	Triclosan	1912002-001	1
Euro OTC	Triclosan	191200201	4
Euro OTC	Triclosan	1912002-01	46
Euro OTC	Triclosan	1912002-02	19
Euro OTC	Triclosan	191200203	2
Euro OTC	Triclosan	1912002-03	40
Euro OTC	Triclosan	1912002-04	21
Euro OTC	Triclosan	19122002-03	1
Euro OTC	Triclosan	20001027-01	1
Euro OTC	Triclosan	2001027-01	28
Euro OTC	Triclosan	2101025-01	1
Euro OTC	Triclosan	2101029	2
Euro OTC	Triclosan	210102901	1
Euro OTC	Triclosan	2101029-01	46
Euro OTC	Triclosan	2101029-02	17
Euro OTC	Triclosan	2101029-03	7
Euro OTC	Triclosan	21011029-02	1
Euro OTC	Triclosan	2206016-01	12
Euro OTC	Triclosan	2206016-02	1
Euro OTC	Triclosan	3078439	1
Euro OTC	Triclosan	4486611	2
Euro OTC	Triclosan	5860088	1
Euro OTC	Triclosan	700228	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Triclosan	CHB1303011-01	1
Euro OTC	Triclosan	K/00111809334	1
Euro UTC	Triclosan	1510045-01	1
Euro/Anzag	Triclosan	1607002-01	1
Euro/Gehe	Triclosan	1602003-01	1
Euro/Noweda	Triclosan	1607002-01	1
Euro/Phoenix	Triclosan	1912002-04	1
Euro/Phoenix	Triclosan	2101029-01	2
Euro/Phönix	Triclosan	160900502	1
Euro/Phönix	Triclosan	170103201	1
Euro/Phönix	Triclosan	1901006	2
Euro/Phönix	Triclosan	1912002-02	1
Euro/Sanacorp	Triclosan	1701032-01	1
Euro/Sanacorp	Triclosan	1912002-01	1
Euro	Triclosan	2001027-01	1
Euroct/Gehe	Triclosan	1510045-01	2
EuRoh/ Gehe	Triclosan	17149821	1
EuRoh/ Gehe	Triclosan	1901006-02	1
EuRoh/ Gehe	Triclosan	191200202	1
EuRoh	Triclosan		1
Euroo/direkt	Triclosan	1705011-01	1
Europ Ots Pharma	Triclosan	13DO2-NO2	1
EurRho/Gehe	Triclosan		1
EurRho/Noweda	Triclosan	1912002-04	1
Fagro/Gehe	Triclosan	13H08-N10	1
Fagro/Sanacorp	Triclosan	TCS0214037	1
Fagron	Triclosan		5
Fagron	Triclosan	10006226	2
Fagron	Triclosan	1006226	1
Fagron	Triclosan	10112014C	1
Fagron	Triclosan	10666066	2
Fagron	Triclosan	106666066	1
Fagron	Triclosan	10J18-N01	2
Fagron	Triclosan	11238004	1
Fagron	Triclosan	11777748	4
Fagron	Triclosan	11A05-N13	2
Fagron	Triclosan	11c21-n05	1
Fagron	Triclosan	11D20-N10	1
Fagron	Triclosan	11h09-n02	1
Fagron	Triclosan	11H09-N02	6
Fagron	Triclosan	11J28-n02	1
Fagron	Triclosan	11J28-N02	4
Fagron	Triclosan	11L19-N11	7
Fagron	Triclosan	1209213402	1
Fagron	Triclosan	1214I03402	1
Fagron	Triclosan	12c21-n05	3
Fagron	Triclosan	12C21-N05	23
Fagron	Triclosan	12G09-N09	4
Fagron	Triclosan	12G09-no9	1
Fagron	Triclosan	12g17-n04	2
Fagron	Triclosan	12G17-n04	2
Fagron	Triclosan	12G17N04	1
Fagron	Triclosan	12G17-N04	30
Fagron	Triclosan	12l06-n01	1
Fagron	Triclosan	12L06-n01	1
Fagron	Triclosan	12L06-N01	35
Fagron	Triclosan	13092012C	1
Fagron	Triclosan	13a11n03	1
Fagron	Triclosan	13A11N03	1
Fagron	Triclosan	13A11-N03	10

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triclosan	13A11-NO3	1
Fagron	Triclosan	13C10-B06-312981	1
Fagron	Triclosan	13d02-n02	1
Fagron	Triclosan	13d02-N02	1
Fagron	Triclosan	13D02N02	1
Fagron	Triclosan	13D02-N02	66
Fagron	Triclosan	13D02-N-02	1
Fagron	Triclosan	13Do2-N02	1
Fagron	Triclosan	13DO2-NO2	1
Fagron	Triclosan	13h08-n10	1
Fagron	Triclosan	13H08N10	2
Fagron	Triclosan	13H08-N10	30
Fagron	Triclosan	13H08-N-10	1
Fagron	Triclosan	13H08-N100450/1231	1
Fagron	Triclosan	13h09-n01	1
Fagron	Triclosan	13H09N01	2
Fagron	Triclosan	13H09-N01	60
Fagron	Triclosan	13H09-N011296/2856	1
Fagron	Triclosan	13H09-No1	1
Fagron	Triclosan	13L18-35-289995	1
Fagron	Triclosan	13L18-B35	12
Fagron	Triclosan	13L18-B35_289995	1
Fagron	Triclosan	13L18-B35-289	1
Fagron	Triclosan	13L18-B35-289983	10
Fagron	Triclosan	13l18-b35-289984	1
Fagron	Triclosan	13L18B35289984	1
Fagron	Triclosan	13L18-B35-289984	5
Fagron	Triclosan	13L18-B35-289985	12
Fagron	Triclosan	13L18-B35-289985	1
Fagron	Triclosan	13L-18-B35-289985	1
Fagron	Triclosan	13L18-B35-289986	5
Fagron	Triclosan	13L18B35289987	1
Fagron	Triclosan	13L18-B35-289987	6
Fagron	Triclosan	13L18-B35-289988	1
Fagron	Triclosan	13L18-B35-289992	2
Fagron	Triclosan	13L18-B35-289993	4
Fagron	Triclosan	13l18-b35-289994	1
Fagron	Triclosan	13L18-B35-289994	7
Fagron	Triclosan	13L18-B35-289995	8
Fagron	Triclosan	14022014C	1
Fagron	Triclosan	14F23-B02	5
Fagron	Triclosan	14F23-B02_295756	1
Fagron	Triclosan	14F23-B02-293852	2
Fagron	Triclosan	14F23-B02-295756	2
Fagron	Triclosan	14f23-b02-295757	1
Fagron	Triclosan	14F23-B02295757	1
Fagron	Triclosan	14F23-B02-295757	6
Fagron	Triclosan	14f23-b02-295758	3
Fagron	Triclosan	14F23B02295758	1
Fagron	Triclosan	14F23-B02-295758	12
Fagron	Triclosan	14F23-B02-295759	9
Fagron	Triclosan	14F23-B02-295760	10
Fagron	Triclosan	14F23-B02-295761	11
Fagron	Triclosan	14F23-B02-295762	3
Fagron	Triclosan	14F23B02295763	1
Fagron	Triclosan	14F23-B02-295763	3
Fagron	Triclosan	14F23-B02-295764	2
Fagron	Triclosan	14F23-B02-295765	6
Fagron	Triclosan	14F23-B02-295947	6
Fagron	Triclosan	14F23-B02-295948	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triclosan	14F23-B02-2959947	1
Fagron	Triclosan	14F23B02300219	1
Fagron	Triclosan	14F23-B02-300219	7
Fagron	Triclosan	14F23-Bo2-295947	1
Fagron	Triclosan	14F-B02-293859	1
Fagron	Triclosan	151010-B06-312984	1
Fagron	Triclosan	15203604	1
Fagron	Triclosan	15301510	1
Fagron	Triclosan	15607-B03-310035	1
Fagron	Triclosan	15C10-806-312981	1
Fagron	Triclosan	15C10-B03-312982	1
Fagron	Triclosan	15C10-B06	5
Fagron	Triclosan	15C10-B06_312980	1
Fagron	Triclosan	15C10B06310031	2
Fagron	Triclosan	15C10-B06-310031	7
Fagron	Triclosan	15C10-B06-310032	4
Fagron	Triclosan	15c10-B06-311161	1
Fagron	Triclosan	15C10B06311161	2
Fagron	Triclosan	15C10-B06-311161	13
Fagron	Triclosan	15c10-b06-312980	1
Fagron	Triclosan	15c10-B06-312980	1
Fagron	Triclosan	15C10-B06-312980	6
Fagron	Triclosan	15c10-b06-312981	1
Fagron	Triclosan	15c10-B06-312981	1
Fagron	Triclosan	15C10-B06-312981	27
Fagron	Triclosan	15C10B06312982	1
Fagron	Triclosan	15C10-B06-312982	14
Fagron	Triclosan	15C10B06312983	1
Fagron	Triclosan	15C10-B06-312983	7
Fagron	Triclosan	15C10-B06-3161	1
Fagron	Triclosan	15C-B06-312982	1
Fagron	Triclosan	15G01-B03-310038	1
Fagron	Triclosan	15G047-B03-0001	1
Fagron	Triclosan	15G07	1
Fagron	Triclosan	15G07-B03	3
Fagron	Triclosan	15G07-B03_310037	1
Fagron	Triclosan	15G07-B03-30037	1
Fagron	Triclosan	15g07-b03-310035	1
Fagron	Triclosan	15G07-B03-310035	9
Fagron	Triclosan	15G07-B03-310036	4
Fagron	Triclosan	15G07B03310037	1
Fagron	Triclosan	15G07-B03-310037	13
Fagron	Triclosan	15G07-B03-310038	6
Fagron	Triclosan	15G07-B03-310039	3
Fagron	Triclosan	15G07B03310040	1
Fagron	Triclosan	15G07-B03-310040	6
Fagron	Triclosan	15G07-B03-310041	1
Fagron	Triclosan	160614	1
Fagron	Triclosan	16084603	1
Fagron	Triclosan	16084614	1
Fagron	Triclosan	1609005-02	2
Fagron	Triclosan	1708025-01	3
Fagron	Triclosan	17081702	1
Fagron	Triclosan	1710025	9
Fagron	Triclosan	17148812	1
Fagron	Triclosan	17149808	1
Fagron	Triclosan	17149814	3
Fagron	Triclosan	17149815	1
Fagron	Triclosan	17149817	2
Fagron	Triclosan	17149819	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Triclosan	17G07-B03-310038	1
Fagron	Triclosan	17K02	1
Fagron	Triclosan	17K02-B06	8
Fagron	Triclosan	17K02-B06-343543	2
Fagron	Triclosan	17K02-B06-343544	10
Fagron	Triclosan	17K02-B06-343545	2
Fagron	Triclosan	17K02-B06343546	1
Fagron	Triclosan	17K02-B06-343546	15
Fagron	Triclosan	17K02-B06-343547	7
Fagron	Triclosan	17K02-B06-343548	9
Fagron	Triclosan	17K02-B06-34547	1
Fagron	Triclosan	18081414	1
Fagron	Triclosan	18082014B	1
Fagron	Triclosan	18253706	2
Fagron	Triclosan	1901006-01	1
Fagron	Triclosan	190282002	1
Fagron	Triclosan	190615A	1
Fagron	Triclosan	1912002-01	1
Fagron	Triclosan	1912002-02	2
Fagron	Triclosan	200315B	1
Fagron	Triclosan	20J30-B03	1
Fagron	Triclosan	20J30-B03-2046408	1
Fagron	Triclosan	20J30-B03-204647	1
Fagron	Triclosan	20J30-B03-204648	1
Fagron	Triclosan	20J30-B03-204649	1
Fagron	Triclosan	20J30-B03-2046-49	1
Fagron	Triclosan	21B25-B02	1
Fagron	Triclosan	21b25-b02-203393	1
Fagron	Triclosan	21B25-B02-203393	2
Fagron	Triclosan	220601601	1
Fagron	Triclosan	22B15-B05-218336	1
Fagron	Triclosan	2513Q-03402	1
Fagron	Triclosan	2901313402	1
Fagron	Triclosan	2914E-03402	1
Fagron	Triclosan	434083	1
Fagron	Triclosan	4394083	1
Fagron	Triclosan	4516I-03402	1
Fagron	Triclosan	5846205	2
Fagron	Triclosan	6012014E	1
Fagron	Triclosan	700228-0005	1
Fagron	Triclosan	90000383	1
Fagron	Triclosan	9000383	2
Fagron	Triclosan	B03-2046409	1
Fagron	Triclosan	C12H7Cl302	1
Fagron	Triclosan	KOO1-1/14/12/823	1
Fagron	Triclosan	TCS0214037	2
Fargon/Fönix	Triclosan	17081725	2
Fargon/Fönix	Triclosan	170817285	1
Fargon/Noweda	Triclosan	18081414	1
Fargon	Triclosan	12C21-NO5	1
fargon	Triclosan	12G17-N04	1
Fargon	Triclosan	13D02-N02	2
Fargon	Triclosan	14F23-B02-295948	1
Fargon	Triclosan	4394403	1
Faron	Triclosan	14F23-B02-300219	2
Fiebig	Triclosan	15C10-B06-312923	1
Fiebig	Triclosan	1607002-01	1
Fiebig	Triclosan	16280811	1
Fiebig	Triclosan	17149813	1
Fiebig	Triclosan	17149814	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fiebig	Triclosan	17149819	1
Fiebig	Triclosan	17149821	1
Fiebig	Triclosan	18081413	2
Fischar/Gehe	Triclosan	13D02-N02	1
Fragron	Triclosan	13D02-N02	1
Fragron	Triclosan	15G07-B03-310040	1
Gaesar & Loretz GmbH	Triclosan	21000427001	2
Gatt-Koller	Triclosan	21J01875	1
GEHE 17.06.2014	Triclosan	14052102	1
GEHE 22.04.2014	Triclosan	13391804	1
Gehe amax	Triclosan	15301503	1
Gehe/Fragon	Triclosan	15C10B06312981	2
Gehe	Triclosan		1
Gehe	Triclosan	11J28-N02	1
Gehe	Triclosan	12145910	1
Gehe	Triclosan	12359104	1
Gehe	Triclosan	12359105	1
Gehe	Triclosan	12359112	1
Gehe	Triclosan	12359114	1
Gehe	Triclosan	12l06-n01	1
Gehe	Triclosan	13391804	2
Gehe	Triclosan	13391811	1
Gehe	Triclosan	13A11-N03	1
Gehe	Triclosan	13D02-N02	1
Gehe	Triclosan	13L18-B35-289992	1
Gehe	Triclosan	14052105	1
Gehe	Triclosan	1408024-01	2
Gehe	Triclosan	14121210	1
Gehe	Triclosan	14121211	1
Gehe	Triclosan	14205904	1
Gehe	Triclosan	14F23B02295947	1
Gehe	Triclosan	14F23-B02-295947	1
Gehe	Triclosan	1505009-01	1
Gehe	Triclosan	16084614	1
Gehe	Triclosan	16280801	2
Gehe	Triclosan	16280808	1
Gehe	Triclosan	16280811	1
Gehe	Triclosan	1701032-01	1
GEHE	Triclosan	1701032-01	1
Gehe	Triclosan	1701032-02	1
GEHE	Triclosan	1701032-02	1
Gehe	Triclosan	1705011-01	1
Gehe	Triclosan	17081710	1
GEHE	Triclosan	17081710	1
Gehe	Triclosan	17149806	1
Gehe	Triclosan	17149809	1
Gehe	Triclosan	17149816	1
Gehe	Triclosan	17149820	2
GEHE	Triclosan	17149824	1
Gehe	Triclosan	18081408	1
Gehe	Triclosan	18253706	1
Gehe	Triclosan	18253709	1
Gehe	Triclosan	18253716	1
GEHE	Triclosan	18253724	1
Gehe	Triclosan	1901006-01	4
Gehe	Triclosan	190100602	1
Gehe	Triclosan	1912002-02	3
gehe	Triclosan	1912002-03	1
Gehe	Triclosan	1912002-03	1
Gehe	Triclosan	2001027-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Triclosan	21000427003	1
GEHE	Triclosan	21000427014	2
Gehe	Triclosan	21000427016	1
Gehe	Triclosan	21000427017	1
Gehe	Triclosan	21000428009	1
gehe	Triclosan	210102901	1
Gehe	Triclosan	2101029-01	3
Gehe	Triclosan	2101029-02	3
Gehe	Triclosan	22060016-01	1
Gehe	Triclosan	2206016-02	1
gehe	Triclosan	23002009001	4
Gehe	Triclosan	Caelo	2
Gehe-Fragon	Triclosan	14F23B02300219	2
Gehe-Fragon	Triclosan	15G07B03310036	2
Geilenkirchen	Triclosan	18253707	1
Geilenkirchen	Triclosan	18253711	1
Geilenkirchen	Triclosan	192709012	1
Gutenberg-Apotheke	Triclosan	13H09-N01	2
Gutenberg-Apotheke	Triclosan	13L18-B35	1
Henry Lamotte/ Noweda	Triclosan	15203606	1
Ichtyhol Gesellschaf…	Triclosan	1701032-02	1
Jenne	Triclosan	18081417	3
Jenne	Triclosan	1912002-03	1
Jenne	Triclosan	20J30-B03	2
Jenne	Triclosan	21000427014	3
Jenne	Triclosan	21000428010	2
Jiangsu EqualChem Co…	Triclosan	1710025	1
Kehr.09.07.2020	Triclosan	2001027-01	1
Kehr	Triclosan	21000427005	1
Kehr	Triclosan	21000427011	3
Kehr	Triclosan	21000427017	3
Kehr	Triclosan	2206016-01	1
Klenk	Triclosan	192709023	1
Klenk	Triclosan	21000428010	1
Klosterring	Triclosan	18081405	1
Kremer/Phönix	Triclosan	15/157/T	1
Krieger/Euro	Triclosan	2101029-01	1
Krieger	Triclosan	12g17-N04	1
Krieger	Triclosan	2206016-01	1
Kumar Organic Produc…	Triclosan	182537001	1
Kumar Organic Products	Triclosan	192709023	1
Kumar Organic/Noweda	Triclosan	15C10-B06	1
Kumar/Noweda	Triclosan		1
Kumar/Noweda	Triclosan	K0011/19/07/337	1
Kumar/Phoenix	Triclosan		2
L12	Triclosan	16280819	1
L12	Triclosan	1628081917181722	1
L12	Triclosan	18081408	1
L30/Alliance	Triclosan	1607002-01	1
Midas	Triclosan	17081714	2
Midas	Triclosan	17081721	1
Midas	Triclosan	17149815	1
Midas	Triclosan	17149819	1
Mvda_23.01.2019	Triclosan	18081416	1
Nachprüfung	Triclosan	AP200710-04	1
Nov	Triclosan	192709011	1
Noveda	Triclosan	18253707	1
now	Triclosan	18257001	1
Nowed 18.12.2014	Triclosan	14121210	2
Noweda 06.12.2019	Triclosan	18253721	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda 15.7.17	Triclosan	16280817	1
Noweda/EuRo	Triclosan	1801049-01	1
Noweda	Triclosan	12359107	1
Noweda	Triclosan	12G17-N04	2
Noweda	Triclosan	13247903	1
noweda	Triclosan	13L18-B35-289985	1
Noweda	Triclosan	1408024-01	1
Noweda	Triclosan	14F23-B02-295765	1
Noweda	Triclosan	15203603	2
Noweda	Triclosan	15203604	1
Noweda	Triclosan	16280818	1
Noweda	Triclosan	1705011-01	1
Noweda	Triclosan	17081703	1
Noweda	Triclosan	17081710	1
Noweda	Triclosan	17081711	1
Noweda	Triclosan	17081714	1
Noweda	Triclosan	17081721	1
Noweda	Triclosan	17081724	1
Noweda	Triclosan	17149801	1
Noweda	Triclosan	17149805	1
Noweda	Triclosan	17149815	1
Noweda	Triclosan	17K02-B06	1
Noweda	Triclosan	17K02-B06-343547	2
Noweda	Triclosan	18081413	1
Noweda	Triclosan	18081417	1
Noweda	Triclosan	182537002	1
Noweda	Triclosan	18253705	1
Noweda	Triclosan	18253708	2
Noweda	Triclosan	18253716	2
Noweda	Triclosan	18253717	1
Noweda	Triclosan	1912002-01	2
Noweda	Triclosan	192709007	1
Noweda	Triclosan	192709011	1
Noweda	Triclosan	192709012	1
Noweda	Triclosan	192709022	2
Noweda	Triclosan	20J30-B03-204648	1
Noweda	Triclosan	210000428009	1
Noweda	Triclosan	21000427007	1
Noweda	Triclosan	21000427008	2
Noweda	Triclosan	21000427011	2
Noweda	Triclosan	21000427017	1
Noweda	Triclosan	21000428004	1
Noweda	Triclosan	21000428009	1
Noweda	Triclosan	21000428015	1
Noweda	Triclosan	21000428020	2
Noweda	Triclosan	2101029-02	1
Noweda	Triclosan	21B25-B02-203393	1
Noweda	Triclosan	2206016-01	1
Ph.Eur 8.0	Triclosan	17081705	1
Phoenix 19.11.14	Triclosan	14121207	1
Phoenix	Triclosan	12003202	1
Phoenix	Triclosan	14205903	1
Phoenix	Triclosan	15C10-B06	1
Phoenix	Triclosan	16084614	1
Phoenix	Triclosan	1609005-02	1
Phoenix	Triclosan	16280809	2
Phoenix	Triclosan	1701032-01	1
Phoenix	Triclosan	1701032-02	1
phoenix	Triclosan	17081707	2
Phoenix	Triclosan	17081709	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Triclosan	17081721	1
Phoenix	Triclosan	17081723	2
Phoenix	Triclosan	17081726	1
Phoenix	Triclosan	17149809	1
Phoenix	Triclosan	17149820	1
Phoenix	Triclosan	17K02-B06-343547	1
Phoenix	Triclosan	18081407	1
Phoenix	Triclosan	18081408	1
Phoenix	Triclosan	18081414	1
Phoenix	Triclosan	18253705	1
Phoenix	Triclosan	18253706	1
Phoenix	Triclosan	18253708	1
Phoenix	Triclosan	18253716	2
Phoenix	Triclosan	18253717	1
Phoenix	Triclosan	18253718	1
Phoenix	Triclosan	18253721	3
Phoenix	Triclosan	1901006-01	1
Phoenix	Triclosan	1912002-02	1
Phoenix	Triclosan	21000427003	1
Phoenix	Triclosan	21000427005	1
Phoenix	Triclosan	21000427014	2
Phoenix	Triclosan	21000428022	1
Phoenix	Triclosan	3417	1
Phöix	Triclosan	21000428022	2
Phönix 27.6.2019	Triclosan	18253705	1
Phönix 5.4.19	Triclosan	18253706	2
Phönix Berlin / Lamotte	Triclosan	17081711	1
Phönix Gotha	Triclosan	13391807	1
Phönix Gotha	Triclosan	1408024-01	2
Phönix Mvda 3.7.2019	Triclosan	18253714	1
Phönix/Caesar&Lorenz…	Triclosan	21000428008	2
Phönix/Caesar&Lorenz…	Triclosan	21000427005	1
Phönix/Eurho	Triclosan	2101029-01	1
Phönix/Fagon	Triclosan	15C10-B06-312981	1
Phönix	Triclosan		1
Phönix	Triclosan	12145908	1
Phönix	Triclosan	12359109	1
Phönix	Triclosan	12359111	1
Phönix	Triclosan	12L06-N01	1
Phönix	Triclosan	13A11-N03	1
Phönix	Triclosan	13H09-N01	1
Phonix	Triclosan	13L18-B35	1
Phönix	Triclosan	13L18-B35-289985	1
Phönix	Triclosan	13L18-B35-289995	2
Phönix	Triclosan	13L8-B35	1
Phönix	Triclosan	1516A-03402	1
Phönix	Triclosan	16280801	1
Phönix	Triclosan	16280811	2
Phönix	Triclosan	17081710	1
phönix	Triclosan	17081712	1
Phönix	Triclosan	17081725	1
Phönix	Triclosan	17149808	1
Phönix	Triclosan	17149815	1
Phönix	Triclosan	17149821	1
Phönix	Triclosan	17k02-b06-343544	1
Phönix	Triclosan	18081415	1
Phönix	Triclosan	182537001	1
Phönix	Triclosan	18253706	1
Phönix	Triclosan	18253718	1
Phönix	Triclosan	18253721	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Triclosan	1912002-01	1
Phönix	Triclosan	1912002-02	1
Phönix	Triclosan	192709004	2
Phönix	Triclosan	192709011	2
Phönix	Triclosan	192709012	1
Phönix	Triclosan	192709018	1
Phönix	Triclosan	192709020	3
phönix	Triclosan	21000427002	1
Phönix	Triclosan	21000427006	1
Phönix	Triclosan	21000427007	1
Phönix	Triclosan	21000427014	2
phönix	Triclosan	21000428010	1
phönix	Triclosan	2101029	1
Phönix	Triclosan	2206016-02	1
Phönix	Triclosan	3180	1
Raben-Apotheke Mildenau	Triclosan	13L18-B35-289984	2
Rondell Apotheke	Triclosan	11965460	1
Röntgen	Triclosan	17K02-B06-343546	1
Röntgen	Triclosan	1801049-01	1
Röntgen	Triclosan	1912002-03	2
Röntgen	Triclosan	2101029-01	2
Sana 06.11.14 EK 3,38	Triclosan	14121209	1
sana corp	Triclosan	12359106	1
sanacorb	Triclosan	18253711	1
Sanacorp 28.05.2019 5,55EUR	Triclosan	1901006-01	1
Sanacorp WE: 30.04.1…	Triclosan	1708025-01	1
Sanacorp WE:05.09.16…	Triclosan	1602003-01	2
Sanacorp	Triclosan		1
Sanacorp	Triclosan	10666066	1
Sanacorp	Triclosan	12359105	2
Sanacorp	Triclosan	12359106	1
Sanacorp	Triclosan	13247904	2
Sanacorp	Triclosan	13391807	2
Sanacorp	Triclosan	13D02-N02	1
Sanacorp	Triclosan	13H09-N01	1
sanacorp	Triclosan	13L18-B35-289987	1
Sanacorp	Triclosan	14052103	1
Sanacorp	Triclosan	14121211	1
Sanacorp	Triclosan	14121215	1
Sanacorp	Triclosan	1505009-01	1
Sanacorp	Triclosan	151004501	1
Sanacorp	Triclosan	17081717	1
Sanacorp	Triclosan	17081725	1
Sanacorp	Triclosan	17149806	1
Sanacorp	Triclosan	17149807	1
Sanacorp	Triclosan	17149808	1
Sanacorp	Triclosan	17149812	1
Sanacorp	Triclosan	17149814	1
Sanacorp	Triclosan	17149821	1
Sanacorp	Triclosan	18081405	2
Sanacorp	Triclosan	18081415	1
Sanacorp	Triclosan	18081416	1
Sanacorp	Triclosan	182537001	1
Sanacorp	Triclosan	182537002	1
Sanacorp	Triclosan	18253702	1
Sanacorp	Triclosan	18253707	1
Sanacorp	Triclosan	18253710	1
Sanacorp	Triclosan	18253711	1
Sanacorp	Triclosan	18253712	1
Sanacorp	Triclosan	18253714	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
sanacorp	Triclosan	18253726	1
sanacorp	Triclosan	1901006-02	1
Sanacorp	Triclosan	1912002-04	1
Sanacorp	Triclosan	192709003	1
Sanacorp	Triclosan	192709022	1
Sanacorp	Triclosan	21000427002	1
Sanacorp	Triclosan	21000427005	1
sanacorp	Triclosan	21000427016	1
Sanacorp	Triclosan	21000428005	1
Sanacorp	Triclosan	2101029-03	1
Sanacorp	Triclosan	2206016-02	1
Sanacorp	Triclosan	26/AKD1	1
Sanacorp	Triclosan	28/AKD4	1
Schulzendorfer-Apotheke	Triclosan	21000427011	1
Sonnenberg-Apotheke	Triclosan	13L18-B35-289995	1
Spangropharm	Triclosan	13D02-V02	1
triclosan	Triclosan	15C10-B06-310032	1
WE:02.04.2016 Sanaco…	Triclosan	15C10-B06-312982	3

- 229 602 spectra from 1514 *Apo-Ident* customers from a total of 48 539 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Triclosan* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Triclosan* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	410	0	152 552
Type B	0	760	0	201 324
Type C	0	6457	8	229 602

The substance/substance group *Triclosan* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5366 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2105 %)
Type C	100.0000 % (> 99.9007 %)	99.8763 % (> 99.8299 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21509	22373	3.92	264.02
21591	22373	5.00	263.35
21615	22373	6.54	262.70
21856	21856	0.00	262.67
22227	22227	0.00	262.97
22373	22373	0.00	263.61
22987	22987	0.00	262.45
23915	22227	12.94	262.25

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Trometamol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20004-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Trometamol; Trometamolum

Special notes

When selecting the *Trometamol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Trometamol	9	8	227

Second-stage model

For differentiation of the substance/substance group *Trometamol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Trometamol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Arginine	120.42	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Trometamol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Trometamol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Trometamol	14050002	21358	40	20140220
Caelo	Trometamol	161688	22629	40	20160615*
Caelo	Trometamol	16168810	23498	40	20160615
Caelo	Trometamol	22000894	26112	40	20220331*
Caelo	Trometamol	22000894	26112SI	20	20220331*
Caelo	Trometamol	22002697	26360	40	20220921*
Caelo	Trometamol	22002697	26360SI	20	20220921*
Caelo	Trometamol	23002408	26972	40	20231012*
Euro OTC	Trometamol	1803016	24063	40	20180320*
Fagron	Trometamol	13E22-N05	20856	40	AR-17-FG-016395-01
Fagron	Trometamol	18A23-B10-351258	24816	40	20180306

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 400 spectra of 11 reference samples from the substance/substance group *Trometamol*. These samples are listed above in the *calibration samples* section. The reference samples come from 9 different batches.

- 152 562 spectra from a total of 2833 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 380 spectra of 10 reference samples from the substance/substance group *Trometamol*.

- Among them are spectra of independent samples from 8 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Trometamol	173208	23787	40
Caelo	Trometamol	190887	25206	40
Caelo	Trometamol	20002276	25640	40
Caelo	Trometamol	23000494	26709	40
Caelo	Trometamol	24000307	27260	40
Euro OTC	Trometamol	2303016	26650	40
Fagron	Trometamol	17A16-B04-334121	23516	40
Fagron	Trometamol	22I20-B05-225357	26465	40
Fagron	Trometamol	17A16-B04-334121	23517	40
Fagron	Trometamol	22I20-B05-225357	26465SI	20

- 201 704 spectra from a total of 4037 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1513 spectra from 758 *Apo-Ident* customers from 235 batches from the substance/substance group *Trometamol*.

- Among them are spectra of independent samples from 225 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Trometamol		1
	Trometamol	2100283014	1
	Trometamol	21002838011	3
	Trometamol	21002838014	4
	Trometamol	22000894006	1
	Trometamol	22002697006	6
	Trometamol	22002697016	9
	Trometamol	23000494005	12
	Trometamol	23000494007	2
	Trometamol	23001254008	3
	Trometamol	23003309002	5
AHC	Trometamol	2300154008	1
AHD	Trometamol	13095910	1
AHD	Trometamol	17320801	1
AHD	Trometamol	18197103	1
Alliance	Trometamol	21002838005	1
Anzag	Trometamol	12113512	1
ANZAG	Trometamol	12113512	1
Anzag	Trometamol	13095911	1
Bartschat	Trometamol	190887007	1
Bombastus	Trometamol	17320811	1
Bombastus	Trometamol	18197103	1
Caelo	Trometamol		6
Caelo	Trometamol	1001312519	1
Caelo	Trometamol	1018U-02519	1
Caelo	Trometamol	11160706	1
Caelo	Trometamol	11160707	1
Caelo	Trometamol	11160711	1
Caelo	Trometamol	11160714	2
Caelo	Trometamol	1119I-02519	1
Caelo	Trometamol	11376005	5
Caelo	Trometamol	11376006	8
Caelo	Trometamol	1180116	1
Caelo	Trometamol	12113502	2
Caelo	Trometamol	12113506	9
Caelo	Trometamol	12113507	3
Caelo	Trometamol	12113510	2
Caelo	Trometamol	12113511	1
Caelo	Trometamol	12113512	10
Caelo	Trometamol	12113515	4
Caelo	Trometamol	13051401	1
Caelo	Trometamol	13095901	10
Caelo	Trometamol	13095902	11
Caelo	Trometamol	13095905	1
Caelo	Trometamol	13095910	5
Caelo	Trometamol	13095911	12
Caelo	Trometamol	13095912	14
Caelo	Trometamol	13095913	3
Caelo	Trometamol	13095915	4
Caelo	Trometamol	13339103	9
Caelo	Trometamol	13339107	8
Caelo	Trometamol	13339108	11
Caelo	Trometamol	1339103	1
Caelo	Trometamol	13C-08-N07	1
Caelo	Trometamol	14050002	7
Caelo	Trometamol	14050003	2
Caelo	Trometamol	14050004	4
Caelo	Trometamol	14050006	1
Caelo	Trometamol	14332402	23
Caelo	Trometamol	14332403	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Trometamol	14332404	1
Caelo	Trometamol	14F19B03304293	1
Caelo	Trometamol	14F19-B03-304293	1
Caelo	Trometamol	150703	1
Caelo	Trometamol	15070304	10
Caelo	Trometamol	15070307	4
Caelo	Trometamol	15070308	29
Caelo	Trometamol	15070309	1
Caelo	Trometamol	15070311	27
Caelo	Trometamol	15094401	15
Caelo	Trometamol	15094404	1
Caelo	Trometamol	15277602	1
Caelo	Trometamol	15377602	25
Caelo	Trometamol	15377604	2
Caelo	Trometamol	15377605	1
Caelo	Trometamol	15377607	31
Caelo	Trometamol	15377611	31
Caelo	Trometamol	15377661	1
Caelo	Trometamol	161013T/15377607	1
Caelo	Trometamol	161668810	1
Caelo	Trometamol	16168801	1
Caelo	Trometamol	16168807	1
Caelo	Trometamol	16168810	40
Caelo	Trometamol	16168810-11417/3	1
Caelo	Trometamol	16168810-6417/1	1
Caelo	Trometamol	16168812	2
Caelo	Trometamol	16168816	2
Caelo	Trometamol	16168819	18
Caelo	Trometamol	16168820	27
Caelo	Trometamol	16168825	2
Caelo	Trometamol	1618810	2
Caelo	Trometamol	16D14-b-09-328729	1
Caelo	Trometamol	17020304	16
Caelo	Trometamol	17053184	1
Caelo	Trometamol	171978	1
Caelo	Trometamol	17197804	30
Caelo	Trometamol	17197806	3
Caelo	Trometamol	17197809	9
Caelo	Trometamol	1719804	1
Caelo	Trometamol	1730804	1
Caelo	Trometamol	173200816	1
Caelo	Trometamol	17320611	1
Caelo	Trometamol	17320801	41
Caelo	Trometamol	17320801/1160518	1
Caelo	Trometamol	17320802	2
Caelo	Trometamol	17320804	44
Caelo	Trometamol	17320810	2
Caelo	Trometamol	17320811	56
Caelo	Trometamol	17320816	33
Caelo	Trometamol	1732816	1
Caelo	Trometamol	17A16-B14	1
Caelo	Trometamol	18041815	1
Caelo	Trometamol	18081503	1
Caelo	Trometamol	181016182	1
Caelo	Trometamol	18197101	14
Caelo	Trometamol	18197103	23
Caelo	Trometamol	18197109	26
Caelo	Trometamol	18197414	1
Caelo	Trometamol	1897103	1
Caelo	Trometamol	18A23-B10-347884	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Trometamol	18A23-B10-349673	1
Caelo	Trometamol	18H13-B04	1
Caelo	Trometamol	190502205	1
Caelo	Trometamol	190887006	2
Caelo	Trometamol	190887007	38
Caelo	Trometamol	190887009	1
Caelo	Trometamol	19088702	3
Caelo	Trometamol	19088705	40
Caelo	Trometamol	19088706	1
Caelo	Trometamol	19197103	1
Caelo	Trometamol	200002276005	1
Caelo	Trometamol	200004247003	1
Caelo	Trometamol	20002276003	1
Caelo	Trometamol	20002276004	1
Caelo	Trometamol	20002276005	34
Caelo	Trometamol	20002276006	28
Caelo	Trometamol	20002276009	1
Caelo	Trometamol	2000424016	1
Caelo	Trometamol	20004247002	1
Caelo	Trometamol	20004247003	18
Caelo	Trometamol	20004247004	1
Caelo	Trometamol	20004247010	3
Caelo	Trometamol	20004247012	1
Caelo	Trometamol	20004247016	17
Caelo	Trometamol	2002276005	1
Caelo	Trometamol	2002276006	1
Caelo	Trometamol	2004247016	1
Caelo	Trometamol	21000487001	50
Caelo	Trometamol	2100048701	1
Caelo	Trometamol	21002838005	15
Caelo	Trometamol	21002838009	1
Caelo	Trometamol	21002838011	9
Caelo	Trometamol	21002838013	1
Caelo	Trometamol	21002838014	2
Caelo	Trometamol	21082013A	1
Caelo	Trometamol	213E-02519	1
Caelo	Trometamol	215I-02519	1
Caelo	Trometamol	22002697006	2
Caelo	Trometamol	22002697016	1
Caelo	Trometamol	23062015B	1
Caelo	Trometamol	26111201	1
Caelo	Trometamol	27111304	1
Caelo	Trometamol	314Q2519	1
Caelo	Trometamol	318A-02519	1
Caelo	Trometamol	3308	1
Caelo	Trometamol	3439	1
Caelo	Trometamol	3713E-02519	1
Caelo	Trometamol	4616M-02519	1
Caelo	Trometamol	5012M-02519	1
Caelo	Trometamol	5315I-02519	1
Caelo	Trometamol	8031301	1
Caelo	Trometamol	8721	1
Caelo	Trometamol	914I-02519	1
Caeolo/Sanacorp	Trometamol	18197101	1
Caesar & Loretz / Sa…	Trometamol	20002276005	1
Caesar & Loretz GmbH…	Trometamol	21002838005	1
Caesar & Loretz GmbH…	Trometamol	21002838005	1
Caesar & Loretz GmbH…	Trometamol	18197101	1
Caesar & Loretz GmbH…	Trometamol	19088705	1
Caesar & Loretz GmbH…	Trometamol	21002838011	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Trometamol	19088705	1
Caesar & Loretz GmbH...	Trometamol	21000487001	2
Caesar & Loretz GmbH...	Trometamol	21002838005	1
Caesar & Loretz GmbH...	Trometamol	22002697016	1
Caesar & Loretz GmbH...	Trometamol	19088705	1
Caesar & Loretz GmbH...	Trometamol	21002838005	1
Caesar & Loretz GmbH...	Trometamol	E300003986	1
Caesar & Loretz GmbH...	Trometamol	11160714	1
Caesar & Loretz GmbH...	Trometamol	13095902	1
Caesar & Loretz GmbH/ AHD	Trometamol	18197108	1
Caesar & Loretz GmbH...	Trometamol	20002276005	1
Caesar & Loretz GmbH...	Trometamol	21002838005	1
Caesar & Loretz GmbH...	Trometamol	190887007	1
Caesar & Loretz GmbH...	Trometamol	20002276005	1
Caesar & Loretz GmbH...	Trometamol	21000487001	1
Caesar & Loretz GmbH/Gehe	Trometamol	190887007	1
Caesar & Loretz GmbH/Gehe	Trometamol	19088705	2
Caesar & Loretz GmbH/Gehe	Trometamol	20002276006	1
Caesar & Loretz GmbH/Gehe	Trometamol	20004247016	1
Caesar & Loretz GmbH...	Trometamol	21000487001	2
Caesar & Loretz GmbH/Kehr	Trometamol	18197103	1
Caesar & Loretz GmbH/L50	Trometamol	21002838005	1
Caesar & Loretz GmbH...	Trometamol	19088705	1
Caesar & Loretz GmbH...	Trometamol	21000487001	1
Caesar & Loretz GmbH...	Trometamol	21002838005	1
Caesar & Loretz GmbH...	Trometamol	21002838011	1
Caesar & Loretz GmbH/Phoe	Trometamol	190887006	1
Caesar & Loretz GmbH...	Trometamol	190887007	1
Caesar & Loretz GmbH...	Trometamol	20002276006	1
Caesar & Loretz GmbH...	Trometamol	21000487001	1
Caesar & Loretz GmbH...	Trometamol	21002838005	1
Caesar & Loretz GmbH...	Trometamol	17320816	1
Caesar & Loretz GmbH...	Trometamol	190887	1
Caesar & Loretz GmbH...	Trometamol	20004247003	2
Caesar & Loretz GmbH...	Trometamol	21000487001	1
Caesar & Loretz GmbH...	Trometamol	22002697006	1
Caesar & Loretz GmbH...	Trometamol	18197103	1
Caesar & Loretz GmbH...	Trometamol	18197103	1
Caesar & Loretz GmbH...	Trometamol	21000487001	1
Caesar & Loretz GmbH	Trometamol	14050003	1
Caesar & Loretz GmbH	Trometamol	17320811	1
Caesar & Loretz GmbH	Trometamol	18197101	2
Caesar & Loretz GmbH	Trometamol	18197103	3
Caesar & Loretz GmbH	Trometamol	18197109	6
Caesar & Loretz GmbH	Trometamol	190887006	3
Caesar & Loretz GmbH	Trometamol	190887007	17
Caesar & Loretz GmbH	Trometamol	19088702	1
Caesar & Loretz GmbH	Trometamol	19088705	11
Caesar & Loretz GmbH	Trometamol	20002276005	10
Caesar & Loretz GmbH	Trometamol	20002276006	4
Caesar & Loretz GmbH	Trometamol	20004247003	7
Caesar & Loretz GmbH	Trometamol	20004247010	2
Caesar & Loretz GmbH	Trometamol	20004247016	5
Caesar & Loretz GmbH	Trometamol	20005576005	1
Caesar & Loretz GmbH	Trometamol	21000487001	20
Caesar & Loretz GmbH	Trometamol	21002838005	9
Caesar & Loretz GmbH	Trometamol	21002838011	5
Caesar & Loretz/Geil...	Trometamol	20004247003	1
Caesar & Loretz/Phoenix	Trometamol	21000487001	1
Caesar & Loretz	Trometamol	16168819	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar / Gehe	Trometamol	15377607	1
Caesar Loretz	Trometamol	190887007	1
Caesar&Loretz	Trometamol	16168820	1
Calo, Hilden/ Phönix	Trometamol	18197109	1
Cealo/Anzag	Trometamol	18197103	1
Cealo	Trometamol	2002276005	1
Celo/Phönix	Trometamol	16168810	1
E300025088	Trometamol	21B15-F03-377086	2
Euro OTC	Trometamol	1203005-02	3
Euro OTC	Trometamol	15070308	1
Euro OTC	Trometamol	15377602	1
Euro OTC	Trometamol	16168810	1
Euro OTC	Trometamol	17197809	2
Euro OTC	Trometamol	17320804	1
Euro OTC	Trometamol	17320816	1
Euro OTC	Trometamol	18197101	1
Fagron	Trometamol	10B26-N05	1
Fagron	Trometamol	12E25-B40	1
Fagron	Trometamol	12I27-N03	1
Fagron	Trometamol	12I27-No3	1
Fagron	Trometamol	12K14-N05	2
Fagron	Trometamol	12k14no5	1
Fagron	Trometamol	13/19-B02	1
Fagron	Trometamol	13/19-B02-286158	3
Fagron	Trometamol	13/19-B02-293595	3
Fagron	Trometamol	13119-B02	1
Fagron	Trometamol	13C08-N07	3
Fagron	Trometamol	13E22-N05	5
Fagron	Trometamol	13I19-B02	1
Fagron	Trometamol	13I19-B02-286158	1
Fagron	Trometamol	13I19-B02-293595	2
Fagron	Trometamol	13l19-B02-286158	1
Fagron	Trometamol	14F19-B03	1
Fagron	Trometamol	14F19-B03-304293	4
Fagron	Trometamol	16(18A23-B10-347884	1
Fagron	Trometamol	16D14-B09	1
Fagron	Trometamol	16d14-b09-328729	1
Fagron	Trometamol	16D14-B09-328729	2
Fagron	Trometamol	17320816	1
Fagron	Trometamol	17A16-B04	2
Fagron	Trometamol	17A16-B04-334121	4
Fagron	Trometamol	17A16-B04-337589	1
Fagron	Trometamol	17A16-B04-340796	4
Fagron	Trometamol	17A16-B04-345550	1
Fagron	Trometamol	18A23-B10-347884	3
Fagron	Trometamol	18A23-B10-349673	5
Fagron	Trometamol	18A23-B10-351258	5
Fagron	Trometamol	18A-23-B10-351258	1
Fagron	Trometamol	18H13-B04-363961	3
Fagron	Trometamol	18H13-B04-363962	1
Fagron	Trometamol	18H13-B04-370289	4
Fagron	Trometamol	20H05-F06-373066	2
Fagron	Trometamol	20H05-F06-373351	2
Fagron	Trometamol	21E18-B03-215278	6
Fagron	Trometamol	21I30-B05	1
Fagron	Trometamol	220728(E300025088)	1
Fagron	Trometamol	294101	1
Fagron	Trometamol	3377086	1
Fagron	Trometamol	610I-02519	1
Fagron	Trometamol	8386E050	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Trometamol	8386H037	1
Fagron	Trometamol	8386J009	2
Fagron	Trometamol	8386K059	1
Fagron	Trometamol	E300003986	2
Fagron	Trometamol	E300021548	3
Fagron	Trometamol	E30021548	1
Fagron	Trometamol	F06-3730607	1
Fagron	Trometamol	TM284375698	1
fargon/gehe	Trometamol	17K23-B04-355709	1
Fargon/Kehr	Trometamol	17A16-B04-337589	1
Fiebig	Trometamol	16168825	1
Fiebig	Trometamol	17320804	1
Gatt-Koller	Trometamol	1801776	1
Gatt-Koller	Trometamol	1804167	1
Gehe 04.11.21 EK:6,97EUR	Trometamol	211105TR	1
Gehe/Fragron	Trometamol	18A23-B10	1
Gehe	Trometamol	11025103	1
Gehe	Trometamol	11160708	1
Gehe	Trometamol	13E22-N05	1
Gehe	Trometamol	15070311	1
Gehe	Trometamol	15377611	1
GEHE	Trometamol	16168810	1
Gehe	Trometamol	17020304	1
Gehe	Trometamol	17A16-B04-345550	1
Gehe	Trometamol	1819701	1
Gehe	Trometamol	18197101	1
GEHE	Trometamol	18A23-B10	1
Gehe	Trometamol	190887007	1
Gehe	Trometamol	19088705	1
Gehe	Trometamol	21000487001	1
Gehe	Trometamol	21002838005	1
Gehe	Trometamol	22002697016	1
Jenne	Trometamol	17320811	1
Klenk	Trometamol	13095902	2
Krieger am 17.08.2018	Trometamol	17320801	1
Merck	Trometamol	8386F017	1
Merck	Trometamol	E300000206913	2
Midas	Trometamol	17197804	1
Nachprüfung	Trometamol	3082019-2	1
Noweda	Trometamol	11376005	1
Noweda	Trometamol	18197101	1
Noweda	Trometamol	19088705	1
Noweda	Trometamol	21002838011	1
Noweda	Trometamol	22002697006	1
Noweda	Trometamol	23001254010	1
Phoenix Hannover	Trometamol	20002276006	1
Phoenix/Cealo	Trometamol	16168825	1
Phoenix	Trometamol	16168819	1
Phoenix	Trometamol	17197804	1
Phoenix	Trometamol	17320804	1
Phoenix	Trometamol	18197109	1
Phoenix	Trometamol	23000494005	1
Phoenix	Trometamol	3039	1
Phoenix	Trometamol	3114	1
Phoenix	Trometamol	3218	1
Phoenix	Trometamol	3409	1
Phönix Gotha	Trometamol	13/19-B02-286158	1
Phönix Gotha	Trometamol	1319-B02-286158	1
Phönix	Trometamol	12113512	1
Phönix	Trometamol	13095912	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Trometamol	14332402	1
Phönix	Trometamol	16168819	1
phönix	Trometamol	17197804	1
Phönix	Trometamol	17197804	1
Phönix	Trometamol	17320804	2
Phönix	Trometamol	17320816	1
Phönix	Trometamol	20002276005	1
PHÖNIX	Trometamol	20004247003	1
phönix	Trometamol	21002838005	1
Phönix	Trometamol	23000494005	1
Post Apotheke	Trometamol	18197101	1
Röntgen	Trometamol	17320801	1
Sanacorp	Trometamol	12113506	1
Sanacorp	Trometamol	13095912	1
Sanacorp	Trometamol	15377602	1
Sanacorp	Trometamol	16168820	1
Sanacorp	Trometamol	17197809	1
Sanacorp	Trometamol	17320804	1
Sanacorp	Trometamol	18197103	1
Sanacorp	Trometamol	21000487001	3
Sanacorp	Trometamol	22002697006	2
Sanacorp	Trometamol	22002697010	1
Sanacorp	Trometamol	23000494005	1
Sanacorp	Trometamol	3686G018	1
Sanacorp	Trometamol	8386H037	1
Sanocorp WE:21.05.16…	Trometamol	15070311	2
Spangro 25.02.2019	Trometamol	18197101	1
vwr chemicals	Trometamol	E300027934	1

- 234 554 spectra from 1515 *Apo-Ident* customers from a total of 49 026 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Trometamol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Trometamol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	400	0	152 562
Type B	0	380	0	201 704
Type C	0	1513	0	234 554

The substance/substance group *Trometamol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.5000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.4211 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 99.6034 %)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20856	20856	0.00	231.05
21358	26112	6.01	212.54
22629	22629	0.00	217.28
23498	22629	10.88	237.86
24063	24063	0.00	225.42
24816	22629	9.67	223.29
26112	26112	0.00	214.44
26360	26360	0.00	207.18
26972	26972	0.00	242.64

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tropicamide**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20598-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tropicamide; Tropicamidum

Special notes

When selecting the *Tropicamide* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tropicamide	6	7	49

Second-stage model

For differentiation of the substance/substance group *Tropicamide* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tropicamide* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	130.67	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tropicamide* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tropicamide*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Tropicamide	2001016	25299	40	20200807*
Euro OTC	Tropicamide	2106001	25709	50	20210720*
Fagron	Tropicamide	14D23-B04-293294	21685	60	AR-15-FG-001641-01
Fagron	Tropicamide	16G19-B05-324829	22885	40	20160905
Fagron	Tropicamide	17J06-B04-341322	23982	40	1807428
Fagron	Tropicamide	21A11-F03-376917	25665	50	20210120

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 280 spectra of 6 reference samples from the substance/substance group *Tropicamide*. These

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 682 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 380 spectra of 11 reference samples from the substance/substance group *Tropicamide*.
- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Audor Pharma	Tropicamide	APFP/TD003/09/17/TR	23983	40
Euro OTC	Tropicamide	2203001	26043	40
Euro OTC	Tropicamide	2204015	26223	40
Euro OTC	Tropicamide	2402034	27209	40
Euro OTC	Tropicamide	2309014	27213	40
Fagron	Tropicamide	17D25-B07-336833	23506	40
Fagron	Tropicamide	18H14-B06-362792	25367	40
Euro OTC	Tropicamide	2106001	25709SI†	10
Euro OTC	Tropicamide	2203001	26043SI	40
Euro OTC	Tropicamide	2204015	26223SI	40
Fagron	Tropicamide	21A11-F03-376917	25665SI†	10

- 201 704 spectra from a total of 4036 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 119 spectra from 30 *Apo-Ident* customers from 51 batches from the substance/substance group *Tropicamide*.
- Among them are spectra of independent samples from 49 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Tropicamide	22D14-B02-220415	1
	Tropicamide	22L08-B03-222105	1
ALH	Tropicamide	15F18-B04-310971	1
Caelo	Tropicamide	17J06-B04-348766	1
Euro OTC	Tropicamide	2001016-01	1
Euro OTC	Tropicamide	2106001-01	2
Fagron	Tropicamide	1/06/2000	1
Fagron	Tropicamide	12F18-N06	4
Fagron	Tropicamide	12l04-n03	1
Fagron	Tropicamide	14D23B04293294	1
Fagron	Tropicamide	14l04-b02-315694	1
Fagron	Tropicamide	14L04B02315694	1
Fagron	Tropicamide	14L04-B02-315694	2
Fagron	Tropicamide	15F18-B04	1
Fagron	Tropicamide	15F18-B04-308977	1
Fagron	Tropicamide	15F18B04312001	1
Fagron	Tropicamide	15F18-B04-312001	1
Fagron	Tropicamide	17D25-B07-336833	6
Fagron	Tropicamide	17J06-B04	2
Fagron	Tropicamide	17J06-B04-341323	5
Fagron	Tropicamide	17J06-B04-343279	2
Fagron	Tropicamide	17J06-B04-348766	4
Fagron	Tropicamide	17J06-B04-352344	2
Fagron	Tropicamide	17J06-B04-354804	3
Fagron	Tropicamide	18H014-B06-357220	1
Fagron	Tropicamide	18H14-B06	1
Fagron	Tropicamide	18H14-B06-357220	5
Fagron	Tropicamide	18H14-B06-359927	6
Fagron	Tropicamide	18H14-B06-362475	3
Fagron	Tropicamide	18H14-B06-362476	8
Fagron	Tropicamide	18H14-B06-362792	1
Fagron	Tropicamide	18H14-B06-362794	7
Fagron	Tropicamide	18H14-B06-362796	1
Fagron	Tropicamide	18H14-B06-363716	1
Fagron	Tropicamide	18H14-B06-369986	1
Fagron	Tropicamide	2/05/1008	1
Fagron	Tropicamide	20021302	1
Fagron	Tropicamide	20C06F03-3699807	1
Fagron	Tropicamide	20C06-F03-369987	3
Fagron	Tropicamide	20C06-F03-371990	2
Fagron	Tropicamide	21H13-B17-213648	2
Fagron	Tropicamide	21H13-B17-216490	6
Fagron	Tropicamide	21J15-B04-216491	2
Fagron	Tropicamide	23071508	1
Fagron	Tropicamide	B06-3627902	2
Fagron	Tropicamide	B06-3627904	1
Fagron	Tropicamide	B06-362794	1
Fagron	Tropicamide	F03-3699807	2
Fagron	Tropicamide	FP/TD/003/09/17	1
Gehe	Tropicamide	15F18-B04	1
Gehe	Tropicamide	15F-18B-04	1
GEHE	Tropicamide	18H14-B06	2
Phoenix	Tropicamide	14L04-B02	2
PHÖNIX	Tropicamide	16G19-B05-324829	1
PHÖNIX	Tropicamide	17J06-B04	5

- 235 948 spectra from 1515 *Apo-Ident* customers from a total of 49 207 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tropicamide* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tropicamide* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	280	0	152 682
Type B	0	380	0	201 704
Type C	0	118	1	235 948

The substance/substance group *Tropicamide* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.8571 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.4211 %)
Type C	100.0000 % (> 99.9007 %)	99.1597 % (> 96.6387 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21685	21685	0.00	221.96
22885	23982	11.19	220.34
23982	23982	0.00	223.29
25299	25299	0.00	221.12
25665	25709	5.24	219.17
25709	25709	0.00	220.19

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tryptophan**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20336-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tryptophan; Tryptophanum

Special notes

When selecting the *Tryptophan* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tryptophan	7	7	11

Second-stage model

For differentiation of the substance/substance group *Tryptophan* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tryptophan* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	194.96	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tryptophan* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tryptophan*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Tryptophan	1506003	21866	60	20150630*
Euro OTC	Tryptophan	1506003	21871	60	20150630*
Euro OTC	Tryptophan	1712006	23876	40	20180105*
Euro OTC	Tryptophan	1910016	24972	40	20191106*
Euro OTC	Tryptophan	2004025	25259	40	20200720*
Euro OTC	Tryptophan	2203027	26051	40	20220413*
Fagron	Tryptophan	14B05-B32-293485	21784	60	AR-15-FG-009473-01
Fagron	Tryptophan	17G19-B01-343931	23998	40	20170919

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 380 spectra of 8 reference samples from the substance/substance group *Tryptophan*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 582 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 320 spectra of 10 reference samples from the substance/substance group *Tryptophan*.

- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Tryptophan	1806006	24144	40
Euro OTC	Tryptophan	1812002	24426	40
Euro OTC	Tryptophan	1906018	24795	40
Euro OTC	Tryptophan	2009041	25421	40
Euro OTC	Tryptophan	2302015	26638	40
Euro OTC	Tryptophan	2401010	27148	30
Fagron	Tryptophan	16E11-B03-322919	23195	40
Euro OTC	Tryptophan	2203027	26051SI†	10
Euro OTC	Tryptophan	2302015	26638SI	20
Euro OTC	Tryptophan	2401010	27148SI	20

- 201 764 spectra from a total of 4037 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 17 spectra from 5 *Apo-Ident* customers from 11 batches from the substance/substance group *Tryptophan*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

- Among them are spectra of independent samples from 11 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Supplier	Substance	Batch	Spectra
Caelo	Tryptophan	131046	1
Euro OTC	Tryptophan	1307004-01	2
Euro OTC	Tryptophan	150600302	1
Euro OTC	Tryptophan	1506003-03	2
Euro OTC	Tryptophan	1712006-01	1
Euro OTC	Tryptophan	180600601	1
Euro OTC	Tryptophan	190601801	1
Euro OTC	Tryptophan	2000402501	1
Euro OTC	Tryptophan	2004025-01	1
Euro OTC	Tryptophan	2203027-01	1
euroct/gehe	Tryptophan	1212010-01	5

- 236 050 spectra from 1515 *Apo-Ident* customers from a total of 49 247 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tryptophan* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tryptophan* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	380	0	152 582
Type B	0	320	0	201 764
Type C	0	17	0	236 050

The substance/substance group *Tryptophan* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.4211 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.1250 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21784	21784	0.00	333.97
21866	21866	0.00	333.90
21871	21871	0.00	332.70
23876	23876	0.00	334.32
23998	24972	4.62	336.17
24972	24972	0.00	334.42
25259	25259	0.00	331.01
26051	26051	0.00	328.86

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tyrosine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21574-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tyrosine; Tyrosinum

Special notes

When selecting the *Tyrosine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tyrosine	6	3	5

Second-stage model

For differentiation of the substance/substance group *Tyrosine* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tyrosine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	108.30	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tyrosine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tyrosine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Tyrosine	2204019	26095	40	20220519*
Euro OTC	Tyrosine	2204019	26095SI	20	20220519*
Fagron	Tyrosine	13G24-N22	21574	60	1411030
Fagron	Tyrosine	16B26-B01-322911	23533	40	20160324
Fagron	Tyrosine	18E15-B02-359934	24692	40	20181001
Fagron	Tyrosine	22B07-B15-221081	26166	40	20220602
Fagron	Tyrosine	22B07-B15-221081	26166SI	20	20220602
Fagron	Tyrosine	22H12-B03-222150	26388	40	20220927
Fagron	Tyrosine	22H12-B03-222150	26388SI	20	20220927

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 320 spectra of 9 reference samples from the substance/substance group *Tyrosine*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 130 spectra of 3 reference samples from the substance/substance group *Tyrosine*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Tyrosine	17B06-B03-338139	24008	40
Fagron	Tyrosine	19I20-F02-365384	25749	50
Fagron	Tyrosine	23B21-B03-227898	27024	40

- 201 954 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5 spectra from 4 *Apo-Ident* customers from 5 batches from the substance/substance group *Tyrosine*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Tyrosine	2204019-01	1
Euro OTC	Tyrosine	L1210050-01	1
Euro OTC	Tyrosine	L1401037	1
Euro OTC	Tyrosine	L1506022-02	1
Euro OTC	Tyrosine	L1506022-05	1

- 236 062 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tyrosine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tyrosine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	130	0	201 954
Type C	0	5	0	236 062

The substance/substance group *Tyrosine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.3846 %)
Type C	100.0000 % (> 99.9009 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21574	21574	0.00	197.64
23533	26095	8.08	204.17
24692	26095	13.56	207.82
26095	26095	0.00	205.38
26166	26095	14.84	209.73
26388	26095	14.78	209.30

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Tyrothricin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20732-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Tyrothricin; Tyrothricinum

Special notes

When selecting the *Tyrothricin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Tyrothricin	3	2	17

Second-stage model

For differentiation of the substance/substance group *Tyrothricin* the following second-stage model is used:

- Submodel 02

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Tyrothricin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Gramicidin	55.49	49.09
⋮	⋮	⋮
Methylprednisolone	>50	71.34
Fluocinolone acetonide	>50	85.25
Betamethasone	>50	98.74
Triamcinolone acetonide	>50	105.21
Prednisolone	>50	111.50
Dexamethasone	>50	131.65

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Tyrothricin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Tyrothricin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Tyrothricin	12K14-N01	20732	40	1509178
Fagron	Tyrothricin	12K14-N01	21683	60	AR-15-FG-001172-01
Fagron	Tyrothricin	14A23-B05-294146	21876	60	AR-15-FG-015005-01
Fagron	Tyrothricin	19C05-B01-370262	25183	40	20200511

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 200 spectra of 4 reference samples from the substance/substance group *Tyrothricin*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

- 152 762 spectra from a total of 2839 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 3 reference samples from the substance/substance group *Tyrothricin*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Tyrothricin	17E09-B03-341231	23742	40
Fagron	Tyrothricin	20L15-F03-376267	26066	40
Fagron	Tyrothricin	20L15-F03-376267	26066SI	10

- 201 994 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 30 spectra from 21 *Apo-Ident* customers from 18 batches from the substance/substance group *Tyrothricin*.

- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Fagron	Tyrothricin	13A14-N04	1
Fagron	Tyrothricin	15A06-B02-3005	1
Fagron	Tyrothricin	15A06-B02-303893	1
Fagron	Tyrothricin	15a06-B02-323005	1
Fagron	Tyrothricin	15A06-B02-323005	5
Fagron	Tyrothricin	17E09-B03	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Tyrothricin	17E09-B03-341231	2
Fagron	Tyrothricin	17E09-B03-350209	1
Fagron	Tyrothricin	17E09-B03-351982	1
Fagron	Tyrothricin	17E09B03352743	1
Fagron	Tyrothricin	17E09-B03-352743	5
Fagron	Tyrothricin	17E09-B03-355400	1
Fagron	Tyrothricin	19C05-B01370262	1
Fagron	Tyrothricin	19C05-B01-370262	1
Fagron	Tyrothricin	19C05-B01-370998	3
Fagron	Tyrothricin	B2500226	2
Parthe Apotheke	Tyrothricin	171/19	1
Sanacorp	Tyrothricin	20L15-F03-376267	1

- 236 037 spectra from 1515 *Apo-Ident* customers from a total of 49 240 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Tyrothricin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Tyrothricin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	90	0	201 994
Type C	0	30	0	236 037

The substance/substance group *Tyrothricin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 93.3333 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 80.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20732	20732	0.00	96.96
21683	21683	0.00	96.85
21876	21876	0.00	90.87
25183	21876	12.97	91.97

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ubidecarenone**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20392-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ubidecarenone; Ubidecarenonum

Special notes

When selecting the *Ubidecarenone* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ubidecarenone	11	16	31

Second-stage model

For differentiation of the substance/substance group *Ubidecarenone* the following second-stage model is used:

- Submodel 05

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ubidecarenone* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	117.19	–
⋮	⋮	⋮
Progesterone	>50	101.30
Fusidic acid	>50	110.40
Spironolactone	>50	117.42
Povidone iodine	>50	134.28
Testosterone propionate	>50	140.33
Povidone	>50	199.47

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ubidecarenone* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ubidecarenone*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Ubidecarenone	14004504	21388	60	AR-15-FG-009220-01
Caelo	Ubidecarenone	17209402	23580	40	20170823
Caelo	Ubidecarenone	17209402	23581	40	20170823
Caelo	Ubidecarenone	172094	23647	35	20170823*
Euro OTC	Ubidecarenone	1205029-01	21247	40	20121009
Euro OTC	Ubidecarenone	1605030	22696	40	20160623*
Euro OTC	Ubidecarenone	1703026	23127	40	20170406*
Euro OTC	Ubidecarenone	1801019	23881	40	20180126*
Euro OTC	Ubidecarenone	2004036	25282	40	20200618*
Euro OTC	Ubidecarenone	2010017	25544	40	20210108*
Fagron	Ubidecarenone	16G26-B01-331742	23161	40	20170110
Fagron	Ubidecarenone	18J24-B01-357225	24688	40	20181121

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 495 spectra of 12 reference samples from the substance/substance group *Ubidecarenone*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 467 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 720 spectra of 21 reference samples from the substance/substance group *Ubidecarenone*.

- Among them are spectra of independent samples from 16 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Ubidecarenone	182298	24281	40
Caelo	Ubidecarenone	21002685002	25975	40
Caelo	Ubidecarenone	22002474	26351	40
Euro OTC	Ubidecarenone	1802025	24074	40
Euro OTC	Ubidecarenone	1804020	24116	40
Euro OTC	Ubidecarenone	1810012	24305	40
Euro OTC	Ubidecarenone	1902030	24630	40
Euro OTC	Ubidecarenone	2003002	25142	40
Euro OTC	Ubidecarenone	2101025	25541	40
Euro OTC	Ubidecarenone	2110011	25894	50
Euro OTC	Ubidecarenone	2205006	26191	40
Euro OTC	Ubidecarenone	2303015	26642	40
Euro OTC	Ubidecarenone	2402030	27215	40
Euro OTC	Ubidecarenone	2410012	27460	40
Fagron	Ubidecarenone	21K09-B08-215716	26075	40
Fagron	Ubidecarenone	23H07-B02-223783	27035	40
Caelo	Ubidecarenone	21002685002	25975SI	10
Caelo	Ubidecarenone	22002474	26351SI	20
Euro OTC	Ubidecarenone	2110011	25894SI	10
Euro OTC	Ubidecarenone	2205006	26191SI	20
Fagron	Ubidecarenone	21K09-B08-215716	26075SI	10

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 364 spectra from a total of 4029 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 46 spectra from 18 *Apo-Ident* customers from 32 batches from the substance/substance group *Ubidecarenone*.

- Among them are spectra of independent samples from 31 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Ubidecarenone	2101025-03	1
Audor Pharma	Ubidecarenone	APSCFQ150614C	1
Audor Pharma	Ubidecarenone	APSZFQ150614C	1
Audor Pharma	Ubidecarenone	APSZFQ170617C	1
Caelo	Ubidecarenone	16G26-B01-344334	2
Caelo	Ubidecarenone	18048401	1
Caesar & Loretz GmbH	Ubidecarenone	20003319001	1
Dr. Behr	Ubidecarenone	WE18020018	1
Euro OTC	Ubidecarenone	1014E-07029	1
Euro OTC	Ubidecarenone	1403020-02	1
Euro OTC	Ubidecarenone	1515M-07029	1
Euro OTC	Ubidecarenone	1605030-01	3
Euro OTC	Ubidecarenone	1801019-01	1
Euro OTC	Ubidecarenone	1802025-01	4
Euro OTC	Ubidecarenone	1804020-01	1
Euro OTC	Ubidecarenone	1810012-01	2
Euro OTC	Ubidecarenone	1902030-01	3
Euro OTC	Ubidecarenone	1902030-02	3
Euro OTC	Ubidecarenone	2110011-01	1
Euro OTC	Ubidecarenone	L1403020-01	1
Fagron	Ubidecarenone	14E12-B06-293861	1
Fagron	Ubidecarenone	14H26-B04-298244	1
Fagron	Ubidecarenone	16B10-B05-327606	1
Fagron	Ubidecarenone	16G26-B01	3
Fagron	Ubidecarenone	18A16-B03	2
Fagron	Ubidecarenone	18a16-b03-351350	1
Fagron	Ubidecarenone	18A16-B03-351350	1
Fagron	Ubidecarenone	18J24-B01	1
Fragon	Ubidecarenone	18J24-B01-362124	1
Sanacorp	Ubidecarenone	2004036-02	1
Sanacorp	Ubidecarenone	2101025-01	1
Sanacorp	Ubidecarenone	51-1911123	1

- 236 021 spectra from 1515 *Apo-Ident* customers from a total of 49 227 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Ubidecarenone* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ubidecarenone* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	495	0	152 467
Type B	0	720	0	201 364
Type C	0	43	3	236 021

The substance/substance group *Ubidecarenone* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7879 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.1667 %)
Type C	100.0000 % (> 99.9007 %)	93.4783 % (> 86.9565 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21247	21388	6.24	134.58
21388	21388	0.00	135.07
22696	22696	0.00	138.77
23127	23127	0.00	136.36
23161	23127	2.25	135.08
23580	22696	4.74	132.30
23581	21388	4.98	132.73
23647	23647	0.00	135.54
23881	23881	0.00	137.67
24688	23881	5.65	135.67
25282	25282	0.00	137.59
25544	25544	0.00	137.52

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all

substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Urea**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20017-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Urea; Ureum

Special notes

When selecting the *Urea* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Urea	11	18	599

Second-stage model

For differentiation of the substance/substance group *Urea* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Urea* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	119.93	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Urea* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Urea*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Urea	15154103	22315	60	20150722
Caelo	Urea	15154103	22315SI	60	20150722
Caelo	Urea	161074	22466	60	20160509*
Caelo	Urea	170216	23033	40	20170202*
Caelo	Urea	18023003	24294	40	20180216
Euro OTC	Urea	1404024-01	21537	60	20140519
Euro OTC	Urea	1601044	22376	40	20160208*
Euro OTC	Urea	1604044	22552	40	20160512*
Euro OTC	Urea	2102002	25549	40	20210205*
Euro OTC	Urea	2301020	26518	40	20230125*
Euro OTC	Urea	2301020	26518SI	40	20230125*
Fagron	Urea	12F25-N05	20712	40	20120724
Fagron	Urea	14I18-B03-303581	22317	60	20141003
Fagron	Urea	14I18-B03-303581	22317SI	60	20141003

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 680 spectra of 14 reference samples from the substance/substance group *Urea*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 282 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 1340 spectra of 33 reference samples from the substance/substance group *Urea*.

- Among them are spectra of independent samples from 18 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Urea	180242	24042	40
Caelo	Urea	180230	24043	40
Caelo	Urea	190316	24550	40
Caelo	Urea	21002313009	25930	40
Caelo	Urea	22002605	26355	40
Caelo	Urea	23001146	26892	40
Caelo	Urea	24001776	27330	40
Euro OTC	Urea	1702023	23156	40
Euro OTC	Urea	1707015	23535	40
Euro OTC	Urea	1804007	24078	40
Euro OTC	Urea	1811012	24340	40
Euro OTC	Urea	1908016	24865	40
Euro OTC	Urea	2004010	25143	40
Euro OTC	Urea	2109001	25829	50
Euro OTC	Urea	2205037	26198	40
Euro OTC	Urea	2309011	26923	40
Fagron	Urea	21L08-B04-219541	26165	40
Fagron	Urea	23C21-B01-228852	27173	40
Caelo	Urea	170216	23033SI†	40
Caelo	Urea	18023003	24294SI†	40
Caelo	Urea	21002313009	25930SI	40
Caelo	Urea	22002605	26355SI	40
Caelo	Urea	23001146	26892SI	40
Caelo	Urea	24001776	27330SI	40
Euro OTC	Urea	1604044	22552SI†	40
Euro OTC	Urea	1702023	23156SI	40
Euro OTC	Urea	1804007	24078SI	40
Euro OTC	Urea	1811012	24340SI	40
Euro OTC	Urea	2109001	25829SI	50

continued on the next page

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Urea	2205037	26198SI	40
Euro OTC	Urea	2309011	26923SI	40
Fagron	Urea	21L08-B04-219541	26165SI	40
Fagron	Urea	23C21-B01-228852	27173SI	40

- 200 744 spectra from a total of 4024 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 6622 spectra from 1345 *Apo-Ident* customers from 617 batches from the substance/substance group *Urea*.
- Among them are spectra of independent samples from 596 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Urea		3
	Urea	12111808	1
	Urea	20003817006	1
	Urea	210002313015	1
	Urea	21002313006	1
	Urea	21002313009	1
	Urea	21002313015	1
	Urea	21002313017	1
	Urea	2109001-01	1
	Urea	21L08-B04-219541	1
	Urea	22002605001	10
	Urea	22002605003	13
	Urea	22002605005	8
	Urea	22002605008	2
	Urea	22002605009	20
	Urea	22002605010	23
	Urea	22002605011	1
	Urea	2200265001	1
	Urea	2200605009	1
	Urea	2205037-01	3
	Urea	2205037-02	2
	Urea	22L02-B12-226179	2
	Urea	23001146001	22
	Urea	23001146002	20
	Urea	23001146003	4
	Urea	23003219004	2
	Urea	23003219005	3
	Urea	23003219010	1
	Urea	23003219011	4
	Urea	23003219012	1
	Urea	2301020-01	2

continued on the next page

[†]These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Urea	2301020-02	1
	Urea	2309011-01	1
	Urea	23J00550	1
	Urea	34567	1
	Urea	B12-2261709	1
	Urea	V034-22022	1
10,68	Urea	23001146003	1
ACM	Urea	KNC0236J16	2
ACM	Urea	KNC0557J15	3
ACM	Urea	KNC1795J14	1
AEP	Urea	22002605001	2
Aep	Urea	23003219011	1
AHC	Urea	15154110	1
AHD	Urea	14E07-B05-293469	1
AHD	Urea	16107428	1
AHD	Urea	18023003	1
AHD	Urea	18023007	2
AHD	Urea	21002313017	1
AHD	Urea	2109001-01	1
AHD	Urea	22002605010	1
AHD	Urea	2205037-01	1
AHD	Urea	22H29-B03-223930	1
AHD	Urea	23001146001	1
AHD	Urea	23003219005	1
AHD	Urea	23003219012	1
AHD	Urea	2301020-01	2
AHD	Urea	2309011-01	1
AHD	Urea	3514E-02544	1
Ahde 27.11.17	Urea	16107422	1
Alliance health	Urea	14E07-B05-297167	1
Alliance Healthcare	Urea	12111823	1
Alliance Healthcare	Urea	190316003	1
Alliance Healthcare	Urea	19031609	1
Alliance Healthcare	Urea	20003817002	1
Alliance Healthcare	Urea	22002605002	1
Alliance Healthcare	Urea	22002605010	1
Alliance	Urea	102002-012	1
Alliance	Urea	21002313006	1
Alliance	Urea	21002313015	1
Alliance	Urea	23001146001	1
Allianz Healthcare	Urea	19031604	1
Anzag / Noweda	Urea	13064206	1
Anzag 17.04.13 ek:6,84EUR	Urea	12111823	1
Anzag/Henry Lamotte	Urea	13-18-B03-303581	1
Anzag	Urea	12111801	1
anzag	Urea	14E07-B05-293469	1
Anzag	Urea	16107411	1
Anzag	Urea	19031614	1
Anzag	Urea	22002605009	1
Anzag	Urea	22002605010	1
Apotheke	Urea	920A-07062	1
Audor Pharma	Urea	2102002-01	2
Audor Pharma	Urea	PU145	1
Beiersdorf AG	Urea	14/18-B03-303576	1
Beiersdorf	Urea	15154112	1
Beyvers/AHD	Urea	15087104	1
Bombastus	Urea	11150721	1
Bombastus	Urea	14107108	1
Bombastus	Urea	15087107	1
Bombastus	Urea	15154104	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Urea	1601044-01	1
Bombastus	Urea	16107424	2
Bombastus	Urea	1707015-01	1
Bombastus	Urea	18023004	1
Bombastus	Urea	18023010	1
Bombastus	Urea	18023012	1
Bombastus	Urea	1804007-01	1
cae	Urea	16107428	1
Caelo	Urea		10
Caelo	Urea	10038587	4
Caelo	Urea	10038593	1
Caelo	Urea	100385993	1
Caelo	Urea	10081208	1
Caelo	Urea	10116	1
Caelo	Urea	10169722	1
Caelo	Urea	10169726	3
Caelo	Urea	1019E-02544	1
Caelo	Urea	1061801	1
Caelo	Urea	107063	1
Caelo	Urea	10823004	1
Caelo	Urea	110087-3	1
Caelo	Urea	1113A-025	1
Caelo	Urea	11150702	2
Caelo	Urea	11150703	1
Caelo	Urea	11150713	1
Caelo	Urea	11150714	1
Caelo	Urea	11150721	1
Caelo	Urea	11150722	3
Caelo	Urea	11150725	3
Caelo	Urea	11150736	4
Caelo	Urea	11150738	1
Caelo	Urea	1171003	1
Caelo	Urea	118023004	1
Caelo	Urea	12111801	4
Caelo	Urea	12111802	8
Caelo	Urea	12111803	1
Caelo	Urea	12111804	4
Caelo	Urea	12111806	5
Caelo	Urea	12111807	5
Caelo	Urea	12111808	9
Caelo	Urea	12111809	12
Caelo	Urea	12111810	14
Caelo	Urea	12111820	11
Caelo	Urea	12111822	16
Caelo	Urea	12111823	9
Caelo	Urea	12111826	6
Caelo	Urea	12111828	20
Caelo	Urea	12111834	3
Caelo	Urea	1211804	1
Caelo	Urea	1211806	1
Caelo	Urea	1211808	1
Caelo	Urea	1211809	1
Caelo	Urea	1211820	1
Caelo	Urea	1222	1
Caelo	Urea	12312478	1
Caelo	Urea	1234	1
Caelo	Urea	12345	1
Caelo	Urea	123456	4
Caelo	Urea	123566	1
Caelo	Urea	1236	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Urea	1241017	1
Caelo	Urea	12L10-N08	3
Caelo	Urea	13042015B	1
Caelo	Urea	13062415	1
Caelo	Urea	1306412	1
Caelo	Urea	13064201	6
Caelo	Urea	13064202	12
Caelo	Urea	13064203	11
Caelo	Urea	13064206	18
Caelo	Urea	13064207	18
Caelo	Urea	13064212	23
Caelo	Urea	13064213	5
Caelo	Urea	13064214	13
Caelo	Urea	13064215	24
Caelo	Urea	13064217	1
Caelo	Urea	1306422	1
Caelo	Urea	13064221	6
Caelo	Urea	13064223	33
Caelo	Urea	13064224	2
Caelo	Urea	13064226	13
Caelo	Urea	13064227	5
Caelo	Urea	13064228	23
Caelo	Urea	13064230	15
Caelo	Urea	13064231	9
Caelo	Urea	13064232	17
Caelo	Urea	13064233	17
Caelo	Urea	13064236	9
Caelo	Urea	13064239	2
Caelo	Urea	13072015B	1
Caelo	Urea	1317B02-287602	1
Caelo	Urea	1364212	1
Caelo	Urea	13E21-N05	1
Caelo	Urea	14/18-B03-303581	2
Caelo	Urea	14011513	1
Caelo	Urea	14064233	1
Caelo	Urea	1407109	1
Caelo	Urea	14107101	13
Caelo	Urea	14107102	27
Caelo	Urea	14107103	8
Caelo	Urea	14107108	10
Caelo	Urea	14107109	21
Caelo	Urea	14107112	20
Caelo	Urea	14107113	17
Caelo	Urea	14107117	10
Caelo	Urea	14107118	8
Caelo	Urea	14107119	25
Caelo	Urea	14107120	10
Caelo	Urea	14107122	17
Caelo	Urea	14107424	1
Caelo	Urea	14107428	1
Caelo	Urea	14197118	1
Caelo	Urea	14E07-B05-289706	1
Caelo	Urea	14E07-B05-293469	1
Caelo	Urea	14I18-B03	1
Caelo	Urea	14I18-B03-303581	1
Caelo	Urea	1501232	1
Caelo	Urea	1508/104	1
Caelo	Urea	15087102	8
Caelo	Urea	15087103	23
Caelo	Urea	15087104	20

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Urea	15087105	12
Caelo	Urea	15087107	20
Caelo	Urea	15087110	26
Caelo	Urea	151154112	1
Caelo	Urea	1514107	1
Caelo	Urea	1514109	1
Caelo	Urea	1514110	2
Caelo	Urea	1514112	1
Caelo	Urea	15145112	1
Caelo	Urea	1515404	1
Caelo	Urea	151541	2
Caelo	Urea	15154101	1
Caelo	Urea	15154103	51
Caelo	Urea	15154104	98
Caelo	Urea	15154107	23
Caelo	Urea	15154109	10
Caelo	Urea	15154110	43
Caelo	Urea	15154111	44
Caelo	Urea	151541111	1
Caelo	Urea	15154112	50
Caelo	Urea	15154113	27
Caelo	Urea	15154116	16
Caelo	Urea	15154116I-020117/1	1
Caelo	Urea	1517E-02544	1
Caelo	Urea	15299506	1
Caelo	Urea	16/13-B02-332593	1
Caelo	Urea	160125/2	1
Caelo	Urea	1604044-01	1
Caelo	Urea	160612/3	1
Caelo	Urea	160620UP	1
Caelo	Urea	1607406	1
Caelo	Urea	1607407	1
Caelo	Urea	1607417	1
Caelo	Urea	1607422	1
Caelo	Urea	161017411	1
Caelo	Urea	1610407	1
Caelo	Urea	1610426	1
Caelo	Urea	161072422	1
Caelo	Urea	16107248	1
Caelo	Urea	161074	2
Caelo	Urea	16107404	1
Caelo	Urea	16107405	13
Caelo	Urea	16107406	23
Caelo	Urea	16107407	42
Caelo	Urea	16107408	2
Caelo	Urea	16107411	40
Caelo	Urea	16107412	100
Caelo	Urea	16107413	11
Caelo	Urea	16107416	19
Caelo	Urea	161074165325	1
Caelo	Urea	16107417	36
Caelo	Urea	16107417-60717/1	1
Caelo	Urea	16107418	35
Caelo	Urea	16107419	26
Caelo	Urea	16107420	60
Caelo	Urea	16107422	51
Caelo	Urea	16107423	12
Caelo	Urea	16107424	89
Caelo	Urea	16107425	7
Caelo	Urea	16107426	27

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Urea	16107427	1
Caelo	Urea	16107428	31
Caelo	Urea	16107429	10
Caelo	Urea	1610743	1
Caelo	Urea	161107417	1
Caelo	Urea	161122-1315	1
Caelo	Urea	16D22-B02-322526	1
Caelo	Urea	16I13-B02-330166	1
Caelo	Urea	16I13-B02-332953	1
Caelo	Urea	17011405	1
Caelo	Urea	1702023-01	3
Caelo	Urea	17021601	5
Caelo	Urea	170509UP/16107407	1
Caelo	Urea	1707015-01	2
Caelo	Urea	17101310	1
Caelo	Urea	17107429	1
Caelo	Urea	17321206	1
Caelo	Urea	18012012	1
Caelo	Urea	1802003	1
Caelo	Urea	180223003	1
Caelo	Urea	18023001	18
Caelo	Urea	18023003	64
Caelo	Urea	18023003-20180830Ma2	1
Caelo	Urea	18023004	164
Caelo	Urea	18023006	74
Caelo	Urea	18023007	46
Caelo	Urea	18023007P-190225-12	1
Caelo	Urea	18023008	1
Caelo	Urea	18023010	75
Caelo	Urea	18023011	106
Caelo	Urea	18023012	113
Caelo	Urea	18023015	107
Caelo	Urea	18023016	8
Caelo	Urea	18023018	55
Caelo	Urea	18023019	6
Caelo	Urea	18023022	6
Caelo	Urea	1802304	1
Caelo	Urea	1802310	1
Caelo	Urea	1802401	1
Caelo	Urea	1802402	1
Caelo	Urea	18024201	58
Caelo	Urea	18024202	58
Caelo	Urea	18024210	1
Caelo	Urea	1803003	1
Caelo	Urea	180322H/18024202	1
Caelo	Urea	1804007-01	1
Caelo	Urea	18109801	1
Caelo	Urea	18203012	1
Caelo	Urea	1823004	1
Caelo	Urea	1824202	1
Caelo	Urea	18G04-B03-353339	1
Caelo	Urea	19016003	1
Caelo	Urea	19031	1
Caelo	Urea	19031314	1
Caelo	Urea	190316001	1
Caelo	Urea	190316002	9
Caelo	Urea	190316003	113
Caelo	Urea	190316003/4520	1
Caelo	Urea	190316003-1	1
Caelo	Urea	190316004	103

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Urea	190316005	3
Caelo	Urea	190316006	43
Caelo	Urea	19031602	1
Caelo	Urea	19031603	8
Caelo	Urea	19031604	86
Caelo	Urea	19031605	61
Caelo	Urea	19031606	51
Caelo	Urea	19031607	4
Caelo	Urea	19031609	49
Caelo	Urea	19031610	45
Caelo	Urea	19031611	7
Caelo	Urea	19031612	1
Caelo	Urea	19031614	50
Caelo	Urea	19031615	58
Caelo	Urea	19031616	8
Caelo	Urea	19031616P-200402-3	1
Caelo	Urea	190318003	1
Caelo	Urea	190319614	1
Caelo	Urea	190321604	1
Caelo	Urea	1903604	1
Caelo	Urea	19041703	1
Caelo	Urea	19061615	1
Caelo	Urea	1908019-01	1
Caelo	Urea	2/20141507	1
Caelo	Urea	200001171004	1
Caelo	Urea	2000011710054	1
Caelo	Urea	200003817013	1
Caelo	Urea	200003817016	1
Caelo	Urea	2000117002	1
Caelo	Urea	20001171002	10
Caelo	Urea	20001171003	11
Caelo	Urea	20001171004	70
Caelo	Urea	200011711002	1
Caelo	Urea	200011711004	1
Caelo	Urea	2000171004	1
Caelo	Urea	2000381	1
Caelo	Urea	20003817001	1
Caelo	Urea	20003817002	28
Caelo	Urea	20003817004	15
Caelo	Urea	20003817005	5
Caelo	Urea	20003817006	7
Caelo	Urea	20003817008	3
Caelo	Urea	20003817010	4
Caelo	Urea	20003817011	16
Caelo	Urea	20003817012	22
Caelo	Urea	20003817013	45
Caelo	Urea	20003817014	7
Caelo	Urea	20003817015	61
Caelo	Urea	20003817016	31
Caelo	Urea	20003817017	1
Caelo	Urea	2000381705	1
Caelo	Urea	20003817061	1
Caelo	Urea	20003817105	1
Caelo	Urea	2000387004	1
Caelo	Urea	2001171004	1
Caelo	Urea	20013100721	1
Caelo	Urea	20031514	1
Caelo	Urea	2003817006	1
Caelo	Urea	200401001	1
Caelo	Urea	2004010-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Urea	20130912-4	1
Caelo	Urea	2016142709	1
Caelo	Urea	20A30-B16-196837	1
Caelo	Urea	210002313009	1
Caelo	Urea	2100231008	1
Caelo	Urea	2100231009	3
Caelo	Urea	2100231017	1
Caelo	Urea	2100231300	1
Caelo	Urea	21002313002	5
Caelo	Urea	21002313004	41
Caelo	Urea	21002313005	4
Caelo	Urea	21002313006	56
Caelo	Urea	21002313007	35
Caelo	Urea	21002313008	6
Caelo	Urea	21002313009	23
Caelo	Urea	21002313013	2
Caelo	Urea	21002313014	27
Caelo	Urea	21002313015	38
Caelo	Urea	21002313016	4
Caelo	Urea	21002313017	25
Caelo	Urea	21003006231	1
Caelo	Urea	2100313007	1
Caelo	Urea	210231304	1
Caelo	Urea	21041802	1
Caelo	Urea	21051304	1
Caelo	Urea	2109212544	1
Caelo	Urea	211100231006	1
Caelo	Urea	21111806	1
Caelo	Urea	2116A-02544	1
Caelo	Urea	22002605001	19
Caelo	Urea	22002605002	3
Caelo	Urea	22002605003	10
Caelo	Urea	22002605005	1
Caelo	Urea	22002605009	2
Caelo	Urea	22002605010	3
Caelo	Urea	2200605001	1
Caelo	Urea	22111305	1
Caelo	Urea	230320/2	1
Caelo	Urea	2324534	1
Caelo	Urea	2416I-02544	1
Caelo	Urea	24882000381715	1
Caelo	Urea	25082015A	1
Caelo	Urea	26071304	1
Caelo	Urea	2738	1
Caelo	Urea	30031304	1
Caelo	Urea	3012A-02544	1
Caelo	Urea	3017E-02544	1
Caelo	Urea	314Q2544	1
Caelo	Urea	3270	1
Caelo	Urea	3357	1
Caelo	Urea	34567890	1
Caelo	Urea	4013Q2544	1
Caelo	Urea	4111M-02544	1
Caelo	Urea	4116M-02544	1
Caelo	Urea	4517M-02544	1
Caelo	Urea	4914I-02544	1
Caelo	Urea	502172207	1
Caelo	Urea	5061410	1
Caelo	Urea	5100	1
Caelo	Urea	5208	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Urea	54215	1
Caelo	Urea	568900	1
Caelo	Urea	6101703	1
Caelo	Urea	62/AKD49	1
Caelo	Urea	63/AKD4	1
Caelo	Urea	813051Up	1
Caelo	Urea	84(18023010)	1
Caelo	Urea	85(18023012)	2
Caelo	Urea	88(20003817002)	1
Caelo	Urea	9031606	1
Caelo	Urea	9031615	1
Caelo	Urea	9240908	1
Caelo	Urea	AKD6	1
Caelo	Urea	Caelo13064233	1
Caelo	Urea	P171218UP08/18	1
Caelo	Urea	Validierungsmessung	1
Caeolo/Gehe	Urea	16107424	1
Caeolo/Noweda	Urea	14107112	1
Caeolo/Noweda	Urea	18023004	1
Caerlo	Urea	18023018	1
Caesar & Lorenz GmbH	Urea	15087107	1
Caesar & Lorenz GmbH	Urea	190316004	1
Caesar & Lorenz GmbH	Urea	19031604	1
Caesar & Loretz / Gehe	Urea	16107428	1
Caesar & Loretz /Phönix	Urea	21002313006	1
Caesar & Loretz GmbH...	Urea	20003817012	1
Caesar & Loretz GmbH...	Urea	15154111	1
Caesar & Loretz GmbH...	Urea	18023010	1
Caesar & Loretz GmbH...	Urea	19031603	1
Caesar & Loretz GmbH...	Urea	20003817012	1
Caesar & Loretz GmbH...	Urea	16107417	1
Caesar & Loretz GmbH...	Urea	17347901	1
Caesar & Loretz GmbH...	Urea	18023003	1
Caesar & Loretz GmbH...	Urea	20003817011	3
Caesar & Loretz GmbH...	Urea	21002313005	1
Caesar & Loretz GmbH...	Urea	22002605010	1
Caesar & Loretz GmbH...	Urea	19031605	1
Caesar & Loretz GmbH...	Urea	21002313002	1
Caesar & Loretz GmbH...	Urea	190316003	1
Caesar & Loretz GmbH...	Urea	19031616	1
Caesar & Loretz GmbH...	Urea	21002313004	1
Caesar & Loretz GmbH...	Urea	21002313007	2
Caesar & Loretz GmbH...	Urea	19031610	1
Caesar & Loretz GmbH...	Urea	190316003	2
Caesar & Loretz GmbH...	Urea	21002313007	1
Caesar & Loretz GmbH...	Urea	20003817015	1
Caesar & Loretz GmbH...	Urea	11150736	1
Caesar & Loretz GmbH...	Urea	12111804	1
Caesar & Loretz GmbH...	Urea	12111810	2
Caesar & Loretz GmbH...	Urea	12111822	1
Caesar & Loretz GmbH...	Urea	12111828	2
Caesar & Loretz GmbH...	Urea	13064206	2
Caesar & Loretz GmbH...	Urea	13064212	3
Caesar & Loretz GmbH/ AEP	Urea	20001171004	1
Caesar & Loretz GmbH...	Urea	19031604	1
Caesar & Loretz GmbH...	Urea	19031615	1
Caesar & Loretz GmbH...	Urea	20001171003	1
Caesar & Loretz GmbH...	Urea	20001171004	1
Caesar & Loretz GmbH...	Urea	19031605	1
Caesar & Loretz GmbH...	Urea	19031606	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Urea	20003817002	1
Caesar & Loretz GmbH...	Urea	20003817013	1
Caesar & Loretz GmbH...	Urea	19031610	2
Caesar & Loretz GmbH...	Urea	20001171003	1
Caesar & Loretz GmbH...	Urea	21002313014	1
Caesar & Loretz GmbH...	Urea	19031606	1
Caesar & Loretz GmbH...	Urea	190316004	1
Caesar & Loretz GmbH...	Urea	21002313020	1
Caesar & Loretz GmbH...	Urea	18023015	1
Caesar & Loretz GmbH...	Urea	19031609	1
Caesar & Loretz GmbH...	Urea	19031610	1
Caesar & Loretz GmbH/A	Urea	21002313007	1
Caesar & Loretz GmbH/AHD	Urea	20003817015	1
Caesar & Loretz GmbH/All	Urea	190316005	1
Caesar & Loretz GmbH...	Urea	20003817016	1
Caesar & Loretz GmbH...	Urea	18023018	1
Caesar & Loretz GmbH...	Urea	190316004	1
Caesar & Loretz GmbH...	Urea	19031611	1
Caesar & Loretz GmbH...	Urea	20003817015	1
Caesar & Loretz GmbH/E	Urea	19031614	1
Caesar & Loretz GmbH/E	Urea	20003817015	1
Caesar & Loretz GmbH...	Urea	18023011	1
Caesar & Loretz GmbH...	Urea	18023015	1
Caesar & Loretz GmbH...	Urea	190316004	3
Caesar & Loretz GmbH...	Urea	19031606	2
Caesar & Loretz GmbH...	Urea	20003817011	1
Caesar & Loretz GmbH...	Urea	21002313006	1
Caesar & Loretz GmbH...	Urea	21002313015	1
Caesar & Loretz GmbH/Gehe	Urea	18023011	1
Caesar & Loretz GmbH/GEHE	Urea	18023011	1
Caesar & Loretz GmbH/Gehe	Urea	190316003	3
Caesar & Loretz GmbH/Gehe	Urea	190316004	1
Caesar & Loretz GmbH/GEHE	Urea	190316004	1
Caesar & Loretz GmbH/Gehe	Urea	190316006	3
Caesar & Loretz GmbH/Gehe	Urea	19031604	1
Caesar & Loretz GmbH/GEHE	Urea	19031604	1
Caesar & Loretz GmbH/Gehe	Urea	19031609	1
Caesar & Loretz GmbH/Gehe	Urea	19031614	4
Caesar & Loretz GmbH/gehe	Urea	19031615	1
Caesar & Loretz GmbH/GEHE	Urea	19031615	1
Caesar & Loretz GmbH/GEHE	Urea	20001171003	2
Caesar & Loretz GmbH/Gehe	Urea	20001171004	1
Caesar & Loretz GmbH/GEHE	Urea	20001171004	2
Caesar & Loretz GmbH/Gehe	Urea	20003817006	2
Caesar & Loretz GmbH/GEHE	Urea	20003817015	1
Caesar & Loretz GmbH/Gehe	Urea	20003817016	1
Caesar & Loretz GmbH/Gehe	Urea	21002313004	2
Caesar & Loretz GmbH/Gehe	Urea	22002605001	1
Caesar & Loretz GmbH...	Urea	20003817008	1
Caesar & Loretz GmbH...	Urea	18023019	1
Caesar & Loretz GmbH...	Urea	190316003	1
Caesar & Loretz GmbH...	Urea	21002313014	1
Caesar & Loretz GmbH...	Urea	20003817016	1
Caesar & Loretz GmbH...	Urea	190316002	1
Caesar & Loretz GmbH...	Urea	19031603	1
Caesar & Loretz GmbH...	Urea	19031610	1
Caesar & Loretz GmbH...	Urea	19031616	1
Caesar & Loretz GmbH/kehr	Urea	18023007	2
Caesar & Loretz GmbH/Kehr	Urea	18023015	1
Caesar & Loretz GmbH/Kehr	Urea	18023019	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH/Kehr	Urea	190316002	1
Caesar & Loretz GmbH/Kehr	Urea	190316003	2
Caesar & Loretz GmbH/Kehr	Urea	19031616	1
Caesar & Loretz GmbH/Kehr	Urea	22002605001	2
Caesar & Loretz GmbH...	Urea	190316004	2
Caesar & Loretz GmbH...	Urea	19031615	1
Caesar & Loretz GmbH...	Urea	20001171004	2
Caesar & Loretz GmbH...	Urea	19031614	1
Caesar & Loretz GmbH...	Urea	20003817016	1
Caesar & Loretz GmbH...	Urea	190316004	1
Caesar & Loretz GmbH...	Urea	190316006	1
Caesar & Loretz GmbH...	Urea	19031615	1
Caesar & Loretz GmbH...	Urea	20001171004	1
Caesar & Loretz GmbH...	Urea	21002313006	1
Caesar & Loretz GmbH/Phoe	Urea	20003817012	1
Caesar & Loretz GmbH...	Urea	190316006	1
Caesar & Loretz GmbH...	Urea	19031606	1
Caesar & Loretz GmbH...	Urea	20003817005	1
Caesar & Loretz GmbH...	Urea	20003817015	1
Caesar & Loretz GmbH...	Urea	21002313015	2
Caesar & Loretz GmbH...	Urea	18023006	1
Caesar & Loretz GmbH...	Urea	190316003	1
Caesar & Loretz GmbH...	Urea	190316004	1
Caesar & Loretz GmbH...	Urea	190316006	1
Caesar & Loretz GmbH...	Urea	19031603	2
Caesar & Loretz GmbH...	Urea	19031611	1
Caesar & Loretz GmbH...	Urea	19031615	1
Caesar & Loretz GmbH...	Urea	20001171003	1
Caesar & Loretz GmbH...	Urea	20003817004	1
Caesar & Loretz GmbH...	Urea	20003817015	4
Caesar & Loretz GmbH...	Urea	21002313004	1
Caesar & Loretz GmbH...	Urea	21002313007	2
Caesar & Loretz GmbH...	Urea	21002313009	1
Caesar & Loretz GmbH...	Urea	21002313015	1
Caesar & Loretz GmbH...	Urea	22002605010	1
Caesar & Loretz GmbH...	Urea	23001146002	2
Caesar & Loretz GmbH...	Urea	190316003	1
Caesar & Loretz GmbH...	Urea	190316004	2
Caesar & Loretz GmbH...	Urea	190316006	1
Caesar & Loretz GmbH...	Urea	19031604	1
Caesar & Loretz GmbH...	Urea	19031606	1
Caesar & Loretz GmbH...	Urea	19031615	1
Caesar & Loretz GmbH...	Urea	20001171004	1
Caesar & Loretz GmbH...	Urea	20003817006	1
Caesar & Loretz GmbH...	Urea	20003817015	2
Caesar & Loretz GmbH...	Urea	21002313007	3
Caesar & Loretz GmbH...	Urea	22002605001	1
Caesar & Loretz GmbH...	Urea	AP210316-01	1
Caesar & Loretz GmbH	Urea	12111822	1
Caesar & Loretz GmbH	Urea	13064206	1
Caesar & Loretz GmbH	Urea	1306421	1
Caesar & Loretz GmbH	Urea	13064223	1
Caesar & Loretz GmbH	Urea	15087103	1
Caesar & Loretz GmbH	Urea	15087105	1
Caesar & Loretz GmbH	Urea	15154104	1
Caesar & Loretz GmbH	Urea	16107411	1
Caesar & Loretz GmbH	Urea	16107417	1
Caesar & Loretz GmbH	Urea	16107419	1
Caesar & Loretz GmbH	Urea	18023004	2
Caesar & Loretz GmbH	Urea	18023006	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Urea	18023007	1
Caesar & Loretz GmbH	Urea	18023008	1
Caesar & Loretz GmbH	Urea	18023010	2
Caesar & Loretz GmbH	Urea	18023011	6
Caesar & Loretz GmbH	Urea	18023012	9
Caesar & Loretz GmbH	Urea	18023013	1
Caesar & Loretz GmbH	Urea	18023015	23
Caesar & Loretz GmbH	Urea	18023016	1
Caesar & Loretz GmbH	Urea	18023018	8
Caesar & Loretz GmbH	Urea	18023019	2
Caesar & Loretz GmbH	Urea	18023022	1
Caesar & Loretz GmbH	Urea	18024201	1
Caesar & Loretz GmbH	Urea	190316002	6
Caesar & Loretz GmbH	Urea	190316003	23
Caesar & Loretz GmbH	Urea	190316004	44
Caesar & Loretz GmbH	Urea	190316005	9
Caesar & Loretz GmbH	Urea	190316006	15
Caesar & Loretz GmbH	Urea	19031602	1
Caesar & Loretz GmbH	Urea	19031603	6
Caesar & Loretz GmbH	Urea	19031604	21
Caesar & Loretz GmbH	Urea	19031605	14
Caesar & Loretz GmbH	Urea	19031606	11
Caesar & Loretz GmbH	Urea	19031607	1
Caesar & Loretz GmbH	Urea	19031608	1
Caesar & Loretz GmbH	Urea	19031609	9
Caesar & Loretz GmbH	Urea	19031610	13
Caesar & Loretz GmbH	Urea	19031611	4
Caesar & Loretz GmbH	Urea	19031612	3
Caesar & Loretz GmbH	Urea	19031614	13
Caesar & Loretz GmbH	Urea	19031615	20
Caesar & Loretz GmbH	Urea	19031616	8
Caesar & Loretz GmbH	Urea	19032609	1
Caesar & Loretz GmbH	Urea	20000092002	1
Caesar & Loretz GmbH	Urea	20001171002	2
Caesar & Loretz GmbH	Urea	20001171003	9
Caesar & Loretz GmbH	Urea	20001171004	32
Caesar & Loretz GmbH	Urea	2000171004	1
Caesar & Loretz GmbH	Urea	20003817002	14
Caesar & Loretz GmbH	Urea	20003817004	3
Caesar & Loretz GmbH	Urea	20003817005	1
Caesar & Loretz GmbH	Urea	20003817006	4
Caesar & Loretz GmbH	Urea	20003817008	2
Caesar & Loretz GmbH	Urea	20003817010	4
Caesar & Loretz GmbH	Urea	20003817011	3
Caesar & Loretz GmbH	Urea	20003817012	6
Caesar & Loretz GmbH	Urea	20003817013	12
Caesar & Loretz GmbH	Urea	20003817014	2
Caesar & Loretz GmbH	Urea	20003817015	28
Caesar & Loretz GmbH	Urea	20003817016	10
Caesar & Loretz GmbH	Urea	21002313001	2
Caesar & Loretz GmbH	Urea	21002313002	2
Caesar & Loretz GmbH	Urea	21002313004	12
Caesar & Loretz GmbH	Urea	21002313005	2
Caesar & Loretz GmbH	Urea	21002313006	18
Caesar & Loretz GmbH	Urea	21002313007	23
Caesar & Loretz GmbH	Urea	21002313008	7
Caesar & Loretz GmbH	Urea	21002313009	8
Caesar & Loretz GmbH	Urea	21002313013	1
Caesar & Loretz GmbH	Urea	21002313014	15
Caesar & Loretz GmbH	Urea	21002313015	21

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Urea	21002313016	1
Caesar & Loretz GmbH	Urea	21002313017	6
Caesar & Loretz GmbH	Urea	220002605001	1
Caesar & Loretz GmbH	Urea	22002605001	10
Caesar & Loretz GmbH	Urea	22002605003	2
Caesar & Loretz GmbH	Urea	22002605009	1
Caesar & Loretz GmbH	Urea	22002605010	1
Caesar & Loretz GmbH7Gehe	Urea	20003817015	1
Caesar & Loretz Hild...	Urea	19031614	1
Caesar & Loretz Hilden	Urea	18023012	1
Caesar & Loretz Hilden	Urea	190316004	1
Caesar & Loretz Hilden	Urea	19031609	1
Caesar & Loretz/AHD	Urea	18023007	2
Caesar & Loretz/Gehe	Urea	19031606	1
Caesar & Loretz/Geil...	Urea	190316003	1
Caesar & Loretz	Urea	16107426	1
Caesar & Loretz	Urea	18023004	2
Caesar & Loretz	Urea	18024201	1
Caesar & Loretz	Urea	20003817002	1
Caesar & Loretz	Urea	20003817015	1
Caesar & Loretz	Urea	21002313006	1
Caesar &Loretz GmbH	Urea	13064203	1
Caesar u Loretz	Urea	12111828	1
Caesar und Loretz Gm...	Urea	18023015	1
Caesar und Loretz GmbH	Urea	20001171004	1
Caesar und Loretz	Urea	16107420	1
Caesar&Loretz GmbH /Anzag	Urea	14107113	1
Caesar&Loretz GmbH /Anzag	Urea	15087110	1
Caesar&Loretz GmbH D...	Urea	12111808	2
Caesar&Loretz GmbH,P...	Urea	16107411	1
Caesar&Loretz GmbH/ ...	Urea	18023001	2
Caesar&Loretz GmbH/Anzag	Urea	13064217	1
Caesar&Loretz GmbH/Anzag	Urea	13064231	1
Caesar&Loretz GmbH	Urea	14107101	1
Caesar&Loretz GmbH	Urea	15154111	1
Caesar&Loretz GmbH	Urea	16107417	1
Caesar&Loretz GmbH	Urea	20003817013	1
Caesar&Loretz GmbH	Urea	21002313004	1
Caesar&loretz,Anzag	Urea	11150738	1
Caesar&loretz,Phoenix	Urea	11150713	1
Caesar&loretz,Phoenix	Urea	12111806	3
Caesar&Loretz/Caesar...	Urea	15154104	1
Caesar&Loretz	Urea	16107428	1
Caesar/Lorenz	Urea	12111822	1
Caesar/Noweda	Urea	12111823	1
Caesar/Noweda	Urea	13064208	1
CaesarLoretz/Gehe	Urea	16107407	1
CaesarLoretz/Gehe	Urea	16107418	1
CaesarLoretz/Gehe	Urea	18023004	1
Caeser & Loretz GmbH/AEP	Urea	21002313006	1
Caeser / Gehe	Urea	15154109	1
Caeser und Loretz GmbH	Urea	18023018	1
Caleo/Noveda	Urea	20003817011	1
Caleo	Urea	18023018	1
Calo/AHD	Urea	15154104	1
Castor/Phönix	Urea	15154104	1
Cealo/AHD	Urea	16107417	1
Cealo/Gehe	Urea	20003817015	1
Cealo/Jenne	Urea	220321(21002313004)	1
Cealo/Phoenix	Urea	18023018	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Cealo/Phönix	Urea	13064231	1
Cealo/Sanacorp	Urea	1804007-01	1
Cealo	Urea	16107416	1
Cealo	Urea	190316003	3
Ceasar & Loretz GmbH...	Urea	16107422	2
Cordes/Noweda	Urea	17021601	1
Dan Pharma	Urea	D08118	1
Delta	Urea	18023004	1
Dr. August Wolff	Urea	13E17N02	1
Dr.Wolff	Urea	1234567	1
Ebert & Jacobi	Urea	15154111	1
Eur	Urea	1707015-01	1
EurHo/ Noweda 11.10.18	Urea	1804007-01	1
EuRho/Noweda	Urea	1707015-01	1
EuRho/Phönix	Urea	2102002-01	1
EuRho	Urea	1212007-01	1
Eurho	Urea	1404024-01	1
EuRho	Urea	150304201	1
EuRho	Urea	1702023-01	1
EuRho	Urea	1707015-01	1
EuRho	Urea	2004010-01	1
Euro / AHD	Urea	1804007-01	1
Euro OTC	Urea		12
Euro OTC	Urea	1008016-01	1
Euro OTC	Urea	1110023-01	1
Euro OTC	Urea	1212007-01	6
Euro OTC	Urea	1212007-02	3
Euro OTC	Urea	13064239	1
Euro OTC	Urea	1404024-01	12
Euro OTC	Urea	14107101	2
Euro OTC	Urea	14107108	1
Euro OTC	Urea	150304201	1
Euro OTC	Urea	1503042-01	26
Euro OTC	Urea	1515404	1
Euro OTC	Urea	15154103	2
Euro OTC	Urea	15154104	3
Euro OTC	Urea	15154107	2
Euro OTC	Urea	160104401	1
Euro OTC	Urea	1601044-01	29
Euro OTC	Urea	160404401	2
Euro OTC	Urea	1604044-01	30
Euro OTC	Urea	16107411	1
Euro OTC	Urea	16107412	3
Euro OTC	Urea	16107428	1
Euro OTC	Urea	16I13-B02-332953	1
Euro OTC	Urea	1702023	1
Euro OTC	Urea	170202301	4
Euro OTC	Urea	1702023-01	30
Euro OTC	Urea	170701501	4
Euro OTC	Urea	1707015-01	41
Euro OTC	Urea	18023006	1
Euro OTC	Urea	18023010	1
Euro OTC	Urea	18023012	1
Euro OTC	Urea	18023015	1
Euro OTC	Urea	18024201	1
Euro OTC	Urea	180400701	1
Euro OTC	Urea	1804007-01	57
Euro OTC	Urea	1804007-02	9
Euro OTC	Urea	1804007-1	1
Euro OTC	Urea	18040701	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Urea	1811012_01	1
Euro OTC	Urea	181101201	1
Euro OTC	Urea	1811012-01	67
Euro OTC	Urea	18110-12-01	1
Euro OTC	Urea	18A24-B07-349015	1
Euro OTC	Urea	19031611	1
Euro OTC	Urea	190801601	2
Euro OTC	Urea	1908016-01	41
Euro OTC	Urea	1908016-16	1
Euro OTC	Urea	1915M-02544	1
Euro OTC	Urea	20003817010	1
Euro OTC	Urea	200401001	2
Euro OTC	Urea	2004010-01	35
Euro OTC	Urea	2004010-02	8
Euro OTC	Urea	2004010-10	1
Euro OTC	Urea	21002313009	1
Euro OTC	Urea	2101002-02	1
Euro OTC	Urea	210200-01	1
Euro OTC	Urea	2102002	1
Euro OTC	Urea	2102002-01	31
Euro OTC	Urea	2102002-02	6
Euro OTC	Urea	2102002-2	1
Euro OTC	Urea	2109001-01	16
Euro OTC	Urea	2205037	1
Euro OTC	Urea	2205037-01	24
Euro OTC	Urea	2205037-02	1
Euro OTC	Urea	220537-01	1
Euro OTC	Urea	72/14	1
Euro OTC	Urea	hcvovo	1
Euro OTC	Urea	UP250171017	1
Euro OTC	Urea	V038-2017	1
Euro OTC	Urea	V076-2016	1
Euro OTC	Urea	V081-2018	3
Euro/Sanacorp	Urea	1707015-01	1
Euro/Sanacorp	Urea	1804007-01	1
Euro/Sanacorp	Urea	1908016-01	2
Fagon/Noweda	Urea	18A24-B07-351975	1
Fagon/Noweda	Urea	19G11-B01	1
Fagon/Noweda	Urea	B01-2014803	1
Fagon/Noweda	Urea	B16-1928504	1
Fagon/Noweda	Urea	V016-2019	1
Fagron	Urea	118900-0001	1
Fagron	Urea	11C25-N01	1
Fagron	Urea	11F24-N16	1
Fagron	Urea	11H01-N08	2
Fagron	Urea	1211822	1
Fagron	Urea	1232255144	1
Fagron	Urea	123456	1
Fagron	Urea	12C20-N05	1
Fagron	Urea	12F25-N05	5
Fagron	Urea	12I04-N06	1
Fagron	Urea	12l04-N06	1
Fagron	Urea	12l10-n08	1
Fagron	Urea	12L10-N08	5
Fagron	Urea	13/17-1302-287602	1
Fagron	Urea	13D03-N01	9
Fagron	Urea	13D03-NO01	1
Fagron	Urea	13E17-N02	1
Fagron	Urea	13E21-N05	2
Fagron	Urea	13J17-B02	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Urea	13J17-B02-287602	2
Fagron	Urea	13J17B02-287604	1
Fagron	Urea	13J17-B02-287604	5
Fagron	Urea	13L20B03	1
Fagron	Urea	13L20-B03_289708	1
Fagron	Urea	13L20-B03-289708	6
Fagron	Urea	14/18-B03-303576	2
Fagron	Urea	14/18B03303581	1
Fagron	Urea	14/18-B03-303581	7
Fagron	Urea	14107117	1
Fagron	Urea	1418b03303581	1
Fagron	Urea	1418B03303581	1
Fagron	Urea	1418-B03-303581	1
Fagron	Urea	14E07B05	3
Fagron	Urea	14E07-B05	8
Fagron	Urea	14E07-B05-289706	1
Fagron	Urea	14E07B05293469	1
Fagron	Urea	14E07-B05-293469	9
Fagron	Urea	14E-07-B05-293469	1
Fagron	Urea	14E07-B05-297165	4
Fagron	Urea	14E07-B05-297167	6
Fagron	Urea	14E07-B07-293469	1
Fagron	Urea	14E8900-0001	1
Fagron	Urea	14I18-B03	4
Fagron	Urea	14I18-B03-303576	7
Fagron	Urea	14I18-B03-303581	3
Fagron	Urea	14l18-B03	1
Fagron	Urea	14l18-B03-0303581	1
Fagron	Urea	15087104	1
Fagron	Urea	15154104	2
Fagron	Urea	15154112	1
Fagron	Urea	16/13-B02	1
Fagron	Urea	16/13-B02-330166	2
Fagron	Urea	16/13-B02-332953	2
Fagron	Urea	1607417	1
Fagron	Urea	16107407	1
Fagron	Urea	16107418	1
Fagron	Urea	16107422	1
Fagron	Urea	1613-B02-328152	2
Fagron	Urea	1613b02332953	1
Fagron	Urea	16D22-802-326481	1
Fagron	Urea	16D22-B02	3
Fagron	Urea	16D22-B02-3221532	1
Fagron	Urea	16D22-B02-322426	1
Fagron	Urea	16D22-B02-322526	6
Fagron	Urea	16D22-B02-322532	5
Fagron	Urea	16D22B02326481	1
Fagron	Urea	16D22-B02-326481	9
Fagron	Urea	16D22-B02-36481	1
Fagron	Urea	16I13-B02	1
Fagron	Urea	16I13-B02-328152	3
Fagron	Urea	16I13-B02-330166	4
Fagron	Urea	16l13-B02-332953	2
Fagron	Urea	1707015-01	1
Fagron	Urea	17D20-B01-335312	1
Fagron	Urea	17H16-B01	3
Fagron	Urea	17H16-B01-340516	1
Fagron	Urea	17H16-B01-342080	4
Fagron	Urea	18023006	1
Fagron	Urea	18023012	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Urea	18023015	2
Fagron	Urea	18024202	1
Fagron	Urea	18A24-B07	3
Fagron	Urea	18A24-B07-346692	5
Fagron	Urea	18A24-B07-347410	1
Fagron	Urea	18A24-B07-3490	1
Fagron	Urea	18A24-B07-349015	4
Fagron	Urea	18A24-B07-351975	8
Fagron	Urea	18A24-B07-352707	3
Fagron	Urea	18-B03-303581	1
Fagron	Urea	18G04-B03	1
Fagron	Urea	18G04-B03-353339	4
Fagron	Urea	18G04-B03-35339	1
Fagron	Urea	18G04-B03-355378	1
Fagron	Urea	18G04-B03-355387	3
Fagron	Urea	19011-B01-194615	1
Fagron	Urea	19E07-B16-162854	2
Fagron	Urea	19E07-B16-190548	3
Fagron	Urea	19e07-b16-192854	1
Fagron	Urea	19E07B16192854	1
Fagron	Urea	19E07-B16-192854	13
Fagron	Urea	19G11_B01_192855	1
Fagron	Urea	19G11-B01_194615	1
Fagron	Urea	19G11-B01-194615	13
Fagron	Urea	20003817015	1
Fagron	Urea	2014162937	3
Fagron	Urea	2016142709	4
Fagron	Urea	2018163455	1
Fagron	Urea	20A30-B16	2
Fagron	Urea	20A30-B16-1968307	1
Fagron	Urea	20A30-b16-196837	1
Fagron	Urea	20A30-B16-196837	7
Fagron	Urea	20A30-B16-196838	2
Fagron	Urea	20E07-801-201907	1
Fagron	Urea	20E07-B01	3
Fagron	Urea	20E07-B01-201455	4
Fagron	Urea	20E07-B01-201483	7
Fagron	Urea	20E07B01201907	2
Fagron	Urea	20E07-B01-201907	9
Fagron	Urea	211120-B02	1
Fagron	Urea	21C16-802	1
Fagron	Urea	21C16-B02	3
Fagron	Urea	21C16-B02_210554	1
Fagron	Urea	21C16-B02-210554	3
Fagron	Urea	21C16-B02-210584	3
Fagron	Urea	21C16B02214451	1
Fagron	Urea	21C16-B02-214451	5
Fagron	Urea	21C16-B02-215566	10
Fagron	Urea	21C16-B02-215659	2
Fagron	Urea	21L08-B04-219541	1
Fagron	Urea	2205037	1
Fagron	Urea	235/12I04-N06	1
Fagron	Urea	2OE07B01201483	1
Fagron	Urea	3613M-02544	1
Fagron	Urea	7L17-NO1	1
Fagron	Urea	9K27-M01	1
Fagron	Urea	B01-2019007	1
Fagron	Urea	B02-2105504	2
Fagron	Urea	B03-303581	1
Fagron	Urea	V018-2021	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Urea	V041-2020	2
Fagron	Urea	V073-2019	1
Fargon/Alliance HC	Urea	14E07-B05-293469	1
Fargon	Urea	14e07-b05-297165	1
Fiebig	Urea	15087103	1
Fiebig	Urea	15154112	1
Fiebig	Urea	16107411	1
Fiebig	Urea	16107417	1
Fiebig	Urea	16107425	1
Fiebig	Urea	16107428	1
Fiebig	Urea	18023004	1
Fiebig	Urea	18023010	1
Fiebig	Urea	18023011	2
Fiebig	Urea	18023018	2
Fiebig	Urea	18024201	1
Finteler Apotheke	Urea	16107417	1
Finze	Urea	1264	1
Gatt-Koller	Urea	1800697	1
Gatt-Koller	Urea	1803268	3
Gehe am 11.10.2017	Urea	16107419	1
Gehe amax	Urea	16107417	1
Gehe amax	Urea	16107422	1
Gehe amax	Urea	18023006	1
Gehe amax	Urea	190316003	1
Gehe amax	Urea	19031614	1
Gehe,05.04.17, 5,30EUR	Urea	16107412	1
Gehe/Fragon	Urea	16D22-B02-326481	1
Gehe	Urea	10038593	1
Gehe	Urea	12111808	1
Gehe	Urea	12111810	1
Gehe	Urea	12111822	1
Gehe	Urea	12111826	1
Gehe	Urea	13064232	1
Gehe	Urea	14107112	1
Gehe	Urea	14107122	1
Gehe	Urea	15087103	1
Gehe	Urea	15087107	2
Gehe	Urea	15154103	1
Gehe	Urea	15154112	1
Gehe	Urea	16107411	2
Gehe	Urea	16107412	3
GEHE	Urea	16107412	1
GEHE	Urea	16107416	1
Gehe	Urea	16107417	1
Gehe	Urea	16107419	1
Gehe	Urea	16107422	3
GEHE	Urea	16107422	1
gehe	Urea	16107425	1
Gehe	Urea	16107425	1
Gehe	Urea	16107428	1
Gehe	Urea	18023004	3
GEHE	Urea	18023006	1
GEHE	Urea	18023007	1
Gehe	Urea	18023011	3
gehe	Urea	18023012	1
Gehe	Urea	18023012	2
Gehe	Urea	18023015	2
Gehe	Urea	18023018	1
gehe	Urea	18024201	1
Gehe	Urea	18024202	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Urea	1804007-01	1
Gehe	Urea	190316002	2
Gehe	Urea	190316004	1
Gehe	Urea	19031604	2
Gehe	Urea	19031606	1
Gehe	Urea	21002313006	1
Gehe	Urea	21002313014	1
Gehe	Urea	210200201	1
GEHE	Urea	2102313014	1
Gehe	Urea	21C16-B02	1
Gehe	Urea	22002605003	1
Gehe	Urea	22002605010	1
GEHE	Urea	2205037-02	1
Gehe	Urea	23001146001	3
Gehe	Urea	2301020-01	2
Gehe	Urea	fgjhghk	1
Geilenkirchen	Urea	18023011	1
Geilenkirchen	Urea	18023015	1
Gutenberg-Apotheke	Urea		1
Gutenberg-Apotheke	Urea	13064227	1
Hänseler	Urea		3
Harnstoff	Urea	20003817016	1
Hirsch	Urea	810811	1
Ichthyol/Noweda	Urea		1
Ichthyol/Phoenix	Urea	15154104	1
ichtxol-Gesellschaft…	Urea	18023010	2
Infectopharm/Phönix	Urea	18023011	1
Jenne 15.11.21, 4,79EUR	Urea	211125	1
Jenne	Urea	18023018	1
Jenne	Urea	23001146001	2
Kehr	Urea	16107418	1
Kehr	Urea	1802007	1
Kehr	Urea	18023004	1
Kehr	Urea	21C16-B02-215566	1
Kehr	Urea	22002605001	1
Kehr	Urea	22002605011	1
Kehr	Urea	2205037-02	1
Kehr	Urea	23001146001	1
Kirsch Pharma GmbH/Noweda	Urea	14E07-B05-293469	1
Kirsch Pharma	Urea	18A24B07346692	1
Krieger	Urea	15154110	1
krieger	Urea	19031604	1
Krieger	Urea	19031610	2
L10	Urea	21C16-B02	1
L12	Urea	16107418	1
L30	Urea	16107407	1
L30	Urea	16107424	1
L30	Urea	18023011	1
Laborchemie Apolda/J…	Urea	12345	1
Lamotte	Urea	19031611	1
Löns Apotheke	Urea	20349	1
Löns Apotheke	Urea	40003	1
Nachprüfung	Urea	2082019-12	1
Nachprüfung	Urea	iu98769879	1
Noveda	Urea	19031610	1
Noveda	Urea	20001171004	1
Noweda 02.08.2019	Urea	18023018	1
Noweda 02.09.2019	Urea	18023019	1
Noweda/KremerGmbH	Urea	13064201	1
Noweda	Urea	11150714	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Urea	13064223	1
Noweda	Urea	14107101	1
Noweda	Urea	15154110	1
Noweda	Urea	15154112	1
Noweda	Urea	16107416	1
Noweda	Urea	16107419	3
Noweda	Urea	16107422	1
Noweda	Urea	18023001	2
Noweda	Urea	18023004	4
Noweda	Urea	18023012	1
Noweda	Urea	18023015	3
Noweda	Urea	18024201	1
Noweda	Urea	18024202	2
Noweda	Urea	19031604	1
Noweda	Urea	19031609	1
Noweda	Urea	19031611	1
Noweda	Urea	20003817004	1
Noweda	Urea	2003817015	1
Noweda	Urea	20E07-B01-201907	1
Noweda	Urea	21002313015	1
Noweda	Urea	21002313017	2
Noweda	Urea	210200-01	1
Noweda	Urea	22002605009	4
NOWEDA	Urea	22002605009	1
Noweda	Urea	22002605010	3
Noweda	Urea	2205037-01	1
Noweda	Urea	2205037-02	1
Noweda	Urea	2301020-01	1
Noweda	Urea	23C21-B01-228853	2
Noweda	Urea	4109M-02544	1
Pala	Urea	18G04-B03-353339	1
Ph.Eur.7.0	Urea	14107109	1
PHOENIX 02.05.2014	Urea	13J17-B02-287602	2
Phoenix 11.09.2017	Urea	16107419	1
Phoenix 17.2.2014	Urea	13064227	1
Phoenix 20.07.2019 4,30EUR	Urea	18023018	1
PHOENIX 29.08.2014	Urea		1
Phoenix 31.07.19	Urea	18023001	1
Phoenix	Urea	13064231	1
Phoenix	Urea	15154113	1
Phoenix	Urea	16107411	1
Phoenix	Urea	16107420	1
Phoenix	Urea	16107424	1
Phoenix	Urea	16107428	1
Phoenix	Urea	18023004	2
Phoenix	Urea	18023006	2
Phoenix	Urea	18023012	1
Phoenix	Urea	18024201	2
Phoenix	Urea	190316004	1
Phoenix	Urea	19031605	1
Phoenix	Urea	19031615	1
Phoenix	Urea	20001171004	1
Phoenix	Urea	20002817013	1
Phoenix	Urea	20003817002	1
Phoenix	Urea	20003817006	1
Phoenix	Urea	20003817012	2
Phoenix	Urea	21002313014	1
Phoenix	Urea	22002605001	1
Phoenix	Urea	23001146002	3
Phoenix	Urea	23003219012	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Urea	3201	1
Phönix Gotha	Urea	1212007-01	1
Phönix Gotha	Urea	13064202	1
Phönix Gotha	Urea	1404024-01	1
Phönix Gotha	Urea	16107417	2
Phönix Gotha	Urea	V096/2012	1
Phönix, Caesar&Loret…	Urea	190316004	3
Phönix/Gehe	Urea	18024201	2
Phönix	Urea	1190316004	1
Phönix	Urea	12111822	1
Phönix	Urea	123456	1
Phönix	Urea	13064207	1
Phönix	Urea	13064215	1
Phönix	Urea	13064223	1
Phönix	Urea	13064236	1
Phönix	Urea	14107109	1
Phönix	Urea	15087110	1
phönix	Urea	15154103	2
phönix	Urea	15154111	1
phönix	Urea	15154112	2
Phönix	Urea	15154113	1
phönix	Urea	16107412	2
Phönix	Urea	16107412	2
Phönix	Urea	16107419	1
phönix	Urea	16107420	1
Phönix	Urea	16107424	1
Phönix	Urea	17H16-B01-342080	1
PHÖNIX	Urea	18023001	1
Phönix	Urea	18023003	2
Phönix	Urea	18023004	1
Phönix	Urea	18023006	1
Phönix	Urea	18023010	1
Phönix	Urea	18023011	1
Phönix	Urea	18023015	1
Phönix	Urea	18023018	2
Phönix	Urea	18024201	1
Phönix	Urea	190316006	1
Phönix	Urea	19031604	2
Phönix	Urea	19031614	2
Phönix	Urea	19031615	1
PHÖNIX	Urea	19031615	1
Phönix	Urea	1908016-01	1
Phönix	Urea	20001171004	2
Phönix	Urea	20003817002	1
Phönix	Urea	20003817012	1
PHÖNIX	Urea	20003817015	1
Phönix	Urea	2004010-01	1
Phönix	Urea	2100231015	1
Phönix	Urea	2102002-01	1
PHönix	Urea	2102002-01	1
Phönix	Urea	22002605001	1
phönix	Urea	22002605003	1
Phönix	Urea	22002605003	1
Phönix	Urea	22002605010	1
Phönix	Urea	23001146002	1
Phönix	Urea	2300114601	1
Phönix	Urea	UP11	1
Phöpnix	Urea	20003817015	1
Px/Phoenix	Urea	18023004	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Raben-Apotheke Mildenau	Urea	13J17-B02-287604	2
Raben-Apotheke Mildenau	Urea	13J17-Bo2-287604	1
Röntgen	Urea	1811012-01	1
Röntgen	Urea	190316003	1
Röntgen	Urea	20003817103	1
sanacorb	Urea	16107424	1
Sanacorp Verbund	Urea	21C16-B02-214451	2
Sanacorp	Urea	1110023-01	1
Sanacorp	Urea	12111808	2
Sanacorp	Urea	12111810	1
Sanacorp	Urea	12111820	1
Sanacorp	Urea	1212007	1
Sanacorp	Urea	13064203	1
Sanacorp	Urea	13064212	1
Sanacorp	Urea	13064223	1
Sanacorp	Urea	1405028-01	1
Sanacorp	Urea	14107102	1
Sanacorp	Urea	14107112	1
Sanacorp	Urea	14107113	1
Sanacorp	Urea	16107417	1
Sanacorp	Urea	16107418	2
Sanacorp	Urea	16107423	1
Sanacorp	Urea	16D22-B02	1
Sanacorp	Urea	1707015-01	2
Sanacorp	Urea	18023004	2
Sanacorp	Urea	18023007	1
Sanacorp	Urea	18023011	1
Sanacorp	Urea	18024202	1
Sanacorp	Urea	1804007-01	2
Sanacorp	Urea	1811012-01	1
Sanacorp	Urea	190316002	1
Sanacorp	Urea	19031604	1
Sanacorp	Urea	19031609	2
Sanacorp	Urea	19031610	1
Sanacorp	Urea	19031615	1
Sanacorp	Urea	1908016-01	1
Sanacorp	Urea	19E07-B16-192854	3
Sanacorp	Urea	20003817015	1
Sanacorp	Urea	2004010-01	2
Sanacorp	Urea	20A30-B16-196837	1
Sanacorp	Urea	21002312001	1
Sanacorp	Urea	21002313007	3
Sanacorp	Urea	21002313016	1
Sanacorp	Urea	210200201	1
Sanacorp	Urea	2102002-01	2
Sanacorp	Urea	21C16-B02-210554	1
Sanacorp	Urea	21C16-B02-214451	1
sanacorp	Urea	22002605009	1
Sanacorp	Urea	22002605009	3
sanacorp	Urea	2301020-01	1
Sanacorp	Urea	2301020-01	1
Sanacorp	Urea	2301020-02	1
Sanacorp	Urea	62/AKD50s	1
Sanacorp	Urea	63/AKD1	1
Sanacorp	Urea	Caelo	1
Sanacorp	Urea	V016-2019	1
SKW Stickstoffwerke	Urea	1804007-01	1
SKW	Urea	1404024-01	1
Spangro 07.02.2014	Urea	13064226	1
Spangro 17.01.2019	Urea	18023007	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Spangro 22.05.2014	Urea	13064230	1
Spangro_07.11.2018	Urea	18023010	1
test	Urea	test	1
THC/Phönix	Urea	18023006	1
Träger	Urea	14107112	1
VDL;05.02.15;10.15EUR	Urea	14107113	1
WE:Phoenix 11.08.16 …	Urea	15154111	1

- 229 445 spectra from 1514 *Apo-Ident* customers from a total of 48 659 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Urea* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Urea* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	680	0	152 282
Type B	0	1340	0	200 744
Type C	0	6619	3	229 445

The substance/substance group *Urea* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.1176 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.5522 %)
Type C	100.0000 % (> 99.9007 %)	99.9547 % (> 99.9094 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20712	22552	4.52	213.73
21537	22466	3.99	216.32
22315	22466	8.10	211.29
22317	22466	4.94	212.45
22376	22376	0.00	214.08
22466	22466	0.00	215.43
22552	22552	0.00	214.24
23033	23033	0.00	212.27
24294	22466	8.25	211.10
25549	25549	0.00	213.32
26518	26518	0.00	212.53

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Ursodeoxycholic acid**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10006311-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Ursodeoxycholic acid; Acidum ursodeoxycholicum

Special notes

When selecting the *Ursodeoxycholic acid* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Ursodeoxycholic acid	4	3	0

Second-stage model

For differentiation of the substance/substance group *Ursodeoxycholic acid* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Ursodeoxycholic acid* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Menthol	81.55	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Ursodeoxycholic acid* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Ursodeoxycholic acid*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Fagron	Ursodeoxycholic acid	20F18-F22-372321	26471	40	240603341
Fagron	Ursodeoxycholic acid	22C09-B03-223073	26472	40	20220526
Fagron	Ursodeoxycholic acid	23E29-B08-228646	26902	40	20230704
Fagron	Ursodeoxycholic acid	23E29-B08-228646	26902SI	20	20230704
Fagron	Ursodeoxycholic acid	UDCA-II-20240633	BR20032	40	20240709*
Fagron	Ursodeoxycholic acid	UDCA-II-20240633	BR20032SI	20	20240709*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 200 spectra of 6 reference samples from the substance/substance group *Ursodeoxycholic acid*.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

These samples are listed above in the *calibration samples* section. The reference samples come from 4 different batches.

- 152 762 spectra from a total of 2838 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 7 reference samples from the substance/substance group *Ursodeoxycholic acid*.
- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Ursodeoxycholic acid	24C07-B17-236823	27265	40
Fagron	Ursodeoxycholic acid	UDCA-II-20240807	BR20033	40
Fagron	Ursodeoxycholic acid	UDCA-II-20240312	BR20034	40
Fagron	Ursodeoxycholic acid	20F18-F22-372321	26471SI†	20
Fagron	Ursodeoxycholic acid	22C09-B03-223073	26472SI†	20
Fagron	Ursodeoxycholic acid	UDCA-II-20240807	BR20033SI	20
Fagron	Ursodeoxycholic acid	UDCA-II-20240312	BR20034SI	20

- 201 884 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 0 spectra from 0 *Apo-Ident* customers from 0 batches from the substance/substance group *Ursodeoxycholic acid*.
- Among them are spectra of independent samples from 0 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.
- 236 067 spectra from 1515 *Apo-Ident* customers from a total of 49 258 batches from a further 722 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Ursodeoxycholic acid* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Ursodeoxycholic acid* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	200	0	152 762
Type B	0	200	0	201 884
Type C	0	0	0	236 067

The substance/substance group *Ursodeoxycholic acid* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9010 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26471	26471	0.00	149.63
26472	26471	53.49	145.85
26902	26471	54.01	145.41
BR20032	BR20032	0.00	142.23

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Valine**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20405-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Valine; Valinum

Special notes

When selecting the *Valine* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Valine	7	13	14

Second-stage model

For differentiation of the substance/substance group *Valine* the following second-stage model is used:

- Submodel 13

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Valine* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Isoleucine	66.13	–
⋮	⋮	⋮
Levocarnitine	>50	36.45
Oxybutynin hydrochloride	>50	118.88
Cyproterone acetate	>50	155.24
Prednicarbate	>50	174.37
Capsaicin	>50	188.18
Sodium citrate	>50	225.46
Amitriptyline hydrochloride	>50	319.49
Norethisterone acetate	>50	355.15
Tetracaine	>50	365.76
Methoxsalen	>50	367.34
Pyridoxal-5-phosphate	>50	398.82
Alfatradiol	>50	467.93
Quinine hydrochloride dihydrate	>50	546.36
Ciprofloxacin hydrochloride	>50	646.78
Heparin sodium	>50	813.07
Triclosan	>50	1728.14
Amifampridine	>50	2472.77
Sucrose	>50	2528.31

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Valine* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Valine*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Valine	1604055	22571	40	20160601*
Euro OTC	Valine	1701026	23131	40	20170222*
Euro OTC	Valine	1904006	24611	40	20190423*
Euro OTC	Valine	1909028	24971	40	20191015*
Euro OTC	Valine	2004021	25169	40	20200505*
Euro OTC	Valine	2006020	25335	40	20200814*
Fagron	Valine	15A14-B07-307756	21953	60	9198

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 300 spectra of 7 reference samples from the substance/substance group *Valine*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.
- 152 662 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 570 spectra of 16 reference samples from the substance/substance group *Valine*.
- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Valine	1609009	22799	40
Euro OTC	Valine	1705017	23426	40
Euro OTC	Valine	1710003	23770	40
Euro OTC	Valine	1712005	23867	40
Euro OTC	Valine	1803017	24091	40
Euro OTC	Valine	1805014	24119	40
Euro OTC	Valine	1809027	24304	40
Euro OTC	Valine	2009046	25422	40
Euro OTC	Valine	2201022	25962	40
Euro OTC	Valine	2205007	26190	40
Euro OTC	Valine	2301008	26574	40
Euro OTC	Valine	2308006	26880	40
Euro OTC	Valine	2403016	27282	40
Euro OTC	Valine	2201022	25962SI	10
Euro OTC	Valine	2205007	26190SI	20
Euro OTC	Valine	2301008	26574SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 514 spectra from a total of 4032 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 19 spectra from 10 *Apo-Ident* customers from 14 batches from the substance/substance group *Valine*.
- Among them are spectra of independent samples from 14 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Valine	1604055-01	2
Euro OTC	Valine	1710003-01	1
Euro OTC	Valine	1805014-01	1
Euro OTC	Valine	1805014-02	2
Euro OTC	Valine	2006020-01	3
Euro OTC	Valine	2009045-03	1
Euro OTC	Valine	2009046-01	2
Euro OTC	Valine	2009046-03	1
Euro OTC	Valine	L1309029-02	1
Fagron	Valine	121259	1
Fagron	Valine	13B13-N05	1
Fagron	Valine	17B27-B03-336205	1
Fagron	Valine	17H14-B04	1
Fagron	Valine	20B12-B02-196844	1

- 236 048 spectra from 1515 *Apo-Ident* customers from a total of 49 244 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Valine* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Valine* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	300	0	152 662
Type B	0	570	0	201 514
Type C	0	18	1	236 048

The substance/substance group *Valine* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.9474 %)
Type C	100.0000 % (> 99.9007 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21953	21953	0.00	99.70
22571	22571	0.00	99.97
23131	23131	0.00	100.82
24611	24611	0.00	97.52
24971	24971	0.00	98.79
25169	25169	0.00	103.69
25335	25335	0.00	102.01

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Vancomycin hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	21748-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Vancomycin hydrochloride; Vancomycini hydrochloridum

Special notes

When selecting the *Vancomycin hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Vancomycin hydrochloride	11	6	5

Second-stage model

For differentiation of the substance/substance group *Vancomycin hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Vancomycin hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	49.09	–
Riboflavin sodium phosphate hydrate	68.36	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Vancomycin hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Vancomycin hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Audor Pharma	Vancomycin hydrochloride	APHAP1609006EV	23532	40	AR-18-FG-000670-01
Euro OTC	Vancomycin hydrochloride	1407047-01	21748	60	AR-15-FG-008950-01
Euro OTC	Vancomycin hydrochloride	1506029	21826	60	AR-15-FG-009077-01
Euro OTC	Vancomycin hydrochloride	1610038	22878	40	20161208*
Euro OTC	Vancomycin hydrochloride	1810013	24325	40	20181029*
Euro OTC	Vancomycin hydrochloride	1908025	24854	40	20190923*
Euro OTC	Vancomycin hydrochloride	2002019	25269	40	20200629*
Euro OTC	Vancomycin hydrochloride	2203002	26048	40	20220419*
Euro OTC	Vancomycin hydrochloride	2402018	27294	40	20240710*
Fagron	Vancomycin hydrochloride	17I18-B08-340944	24010	40	20171109
Fagron	Vancomycin hydrochloride	18L18-B02-359948	24696	40	20190207

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 480 spectra of 11 reference samples from the substance/substance group *Vancomycin hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 11 different batches.

- 152 482 spectra from a total of 2831 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 290 spectra of 9 reference samples from the substance/substance group *Vancomycin hydrochloride*.

- Among them are spectra of independent samples from 6 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Vancomycin hydrochloride	1604037	22891	40
Euro OTC	Vancomycin hydrochloride	1812005	24421	40
Euro OTC	Vancomycin hydrochloride	1902014	24492	40
Euro OTC	Vancomycin hydrochloride	2211001	26525	40
Fagron	Vancomycin hydrochloride	22G01-B07-221838	26383	40
Fagron	Vancomycin hydrochloride	23G06-B01-230986	26988	40
Euro OTC	Vancomycin hydrochloride	2203002	26048SI†	10
Euro OTC	Vancomycin hydrochloride	2211001	26525SI	20
Fagron	Vancomycin hydrochloride	22G01-B07-221838	26383SI	20

- 201 794 spectra from a total of 4038 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 7 spectra from 2 *Apo-Ident* customers from 5 batches from the substance/substance group *Vancomycin hydrochloride*.
- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Euro OTC	Vancomycin hydrochloride	1902014-01	2
Euro OTC	Vancomycin hydrochloride	2101015-01	1
Fagron	Vancomycin hydrochloride	20G16-F07	1
Fagron	Vancomycin hydrochloride	21G16-B01-217709	2
Fagron	Vancomycin hydrochloride	21G16-B01	1

- 236 060 spectra from 1515 *Apo-Ident* customers from a total of 49 253 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Vancomycin hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Vancomycin hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	480	0	152 482
Type B	0	290	0	201 794
Type C	0	5	2	236 060

The substance/substance group *Vancomycin hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.7500 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.9310 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21748	21748	0.00	110.62
21826	21826	0.00	89.33
22878	22878	0.00	101.61
23532	23532	0.00	88.17
24010	23532	27.60	93.54
24325	24325	0.00	88.94
24696	26048	11.63	102.04
24854	24854	0.00	114.10
25269	25269	0.00	102.24
26048	26048	0.00	108.49
27294	27294	0.00	96.26

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Vanillin**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20204-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Vanillin; Vanillinum

Special notes

When selecting the *Vanillin* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Vanillin	6	4	60

Second-stage model

For differentiation of the substance/substance group *Vanillin* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Vanillin* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Sodium cromoglicate	98.90	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Vanillin* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Vanillin*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Vanillin	14044413	21737	60	20140227
Caelo	Vanillin	15135302	21924	60	AR-17-FG-022168-03
Caelo	Vanillin	160895	22484	60	20160421*
Caelo	Vanillin	191201	24719	40	20190515*
Caelo	Vanillin	22001135	26109	40	20220408*
Fagron	Vanillin	13J01-N07	21738	60	20130926

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 320 spectra of 6 reference samples from the substance/substance group *Vanillin*. These samples

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 642 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 200 spectra of 6 reference samples from the substance/substance group *Vanillin*.
- Among them are spectra of independent samples from 4 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Vanillin	171172	23308	40
Caelo	Vanillin	17117201	23561	40
Caelo	Vanillin	173088	23805	40
Caelo	Vanillin	23003197	27118	40
Caelo	Vanillin	22001135	26109SI†	20
Caelo	Vanillin	23003197	27118SI	20

- 201 884 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 233 spectra from 179 *Apo-Ident* customers from 64 batches from the substance/substance group *Vanillin*.
- Among them are spectra of independent samples from 60 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

Supplier	Substance	Batch	Spectra
	Vanillin	21001092003	1
	Vanillin	22001135004	4
	Vanillin	22001135012	1
	Vanillin	23003197003	1
Anzag	Vanillin	12H09-N06	1
Anzag	Vanillin	16089508	1
Caelo	Vanillin		1
Caelo	Vanillin	10066811	1
Caelo	Vanillin	10066830	1
Caelo	Vanillin	1089501	1
Caelo	Vanillin	112901	1
Caelo	Vanillin	12071401	1
Caelo	Vanillin	12079407	2
Caelo	Vanillin	12079410	2
Caelo	Vanillin	12079412	2
Caelo	Vanillin	12079417	1
Caelo	Vanillin	12079424	2
Caelo	Vanillin	12079428	1
Caelo	Vanillin	14044419	3
Caelo	Vanillin	15135302	2
Caelo	Vanillin	1514006	1
Caelo	Vanillin	15154006	1
Caelo	Vanillin	15154014	4
Caelo	Vanillin	15154017	2
Caelo	Vanillin	15154020	6
Caelo	Vanillin	15227317	1
Caelo	Vanillin	16089501	3
Caelo	Vanillin	16089506	12
Caelo	Vanillin	16089508	3
Caelo	Vanillin	17117201	2
Caelo	Vanillin	17117207	19
Caelo	Vanillin	17117208	3
Caelo	Vanillin	18073501	9
Caelo	Vanillin	18073506	3
Caelo	Vanillin	18073507	7
Caelo	Vanillin	18073509	4
Caelo	Vanillin	18073511	5
Caelo	Vanillin	18073515	5
Caelo	Vanillin	191201005	9
Caelo	Vanillin	19120102	9
Caelo	Vanillin	20000477003	4
Caelo	Vanillin	20003608002	4
Caelo	Vanillin	20003608006	4
Caelo	Vanillin	2000477003	1
Caelo	Vanillin	21001092003	5
Caelo	Vanillin	21001092009	5
Caelo	Vanillin	211029	1
Caelo	Vanillin	2200135004	2
Caelo	Vanillin	250220004773	1
Caelo	Vanillin	4216I-02548	1
Caelo	Vanillin	90961269	1
Caesar & Loretz GmbH...	Vanillin	21001092003	1
Caesar & Loretz GmbH...	Vanillin	18073515	1
Caesar & Loretz GmbH...	Vanillin	18073507	1
Caesar & Loretz GmbH...	Vanillin	10066830	1
Caesar & Loretz GmbH...	Vanillin	12079401	1
Caesar & Loretz GmbH...	Vanillin	12079412	1
Caesar & Loretz GmbH	Vanillin	18073511	1
Caesar & Loretz GmbH	Vanillin	18073515	1
Caesar & Loretz GmbH	Vanillin	191201005	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Vanillin	20000477003	1
Caesar & Loretz GmbH	Vanillin	20003608002	3
Caesar & Loretz GmbH	Vanillin	20003608006	1
Caesar & Loretz GmbH	Vanillin	21001092003	2
Caesar & Loretz GmbH	Vanillin	21001092009	4
Caesar & Loretz GmbH	Vanillin	22001135011	1
Caesar & Loretz/Geil...	Vanillin	191201005	1
Caleo / Phoenix	Vanillin	20000477003	1
Dr.Hollborn	Vanillin	6082015	1
Fagron	Vanillin	11G28-N09	1
Fagron	Vanillin	12D02-N03	1
Fagron	Vanillin	12H09-N06	2
Fagron	Vanillin	13J01-N07	6
Fagron	Vanillin	14G02-B99-296988	1
Fagron	Vanillin	18073501	1
Fagron	Vanillin	232050-0004	1
Fagron	Vanillin	314Q2548	1
Fagron	Vanillin	8L05-N07	1
fargron	Vanillin	13/01-N07	1
Finteler Apotheke	Vanillin	17117201	1
Gatt-Koller	Vanillin	201770800	1
Gehe/Noweda	Vanillin	15154006	1
Gehe	Vanillin	12079412	1
Gehe	Vanillin	16089506	1
Gehe	Vanillin	20000477003	1
Hedinger/Ebert	Vanillin	13A30-N10	1
Jenne	Vanillin	18073501	1
Klosterring	Vanillin	17117207	1
L10	Vanillin	18073506	1
L12	Vanillin	16089508	1
L12	Vanillin	17117201	1
L12	Vanillin	18073501	1
labor	Vanillin	101010101	1
Noweda	Vanillin	18073501	1
Phoenix	Vanillin	21001092003	1
Reagenz Ph.Eur.	Vanillin		1
Rhodia GmbH/Noweda	Vanillin	12D02-N03	1
Sanacorp	Vanillin	12H09-N06	1
Sanacorp	Vanillin	20000477003	1

- 235 834 spectra from 1515 *Apo-Ident* customers from a total of 49 197 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Vanillin* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Vanillin* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	320	0	152 642
Type B	0	200	0	201 884
Type C	0	232	1	235 834

The substance/substance group *Vanillin* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.1250 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.0000 %)
Type C	100.0000 % (> 99.9007 %)	99.5708 % (> 98.2833 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21737	21924	2.90	197.24
21738	21924	3.96	201.46
21924	21924	0.00	189.07
22484	22484	0.00	205.79
24719	24719	0.00	208.48
26109	26109	0.00	221.14

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Waxes / Fats**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20865-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Waxes / Fats; Adeps solidus; Adeps solidus W35; Beeswax, white; Beeswax, yellow; Cera alba; Cera flava; Cetyl palmitate; Cetylis palmitas; Cocoa butter; Hard fat; Hard fat W35; Microcrystalline wax; Natrii laurilsulfas; Paraffin, hard; Paraffin, microcrystalline; Paraffina microcristallina; Paraffinum solidum; Sodium dodecyl sulfate; Sodium dodecyl sulphate; Theobromatis oleum

Special notes

When selecting the *Waxes / Fats* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Waxes / Fats	59	49	1135

Second-stage model

For differentiation of the substance/substance group *Waxes / Fats* the following second-stage model is used:

- Submodel 01

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Waxes / Fats* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Magnesium stearate	67.37	21.80

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Waxes / Fats* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Waxes / Fats*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Beeswax, white	13378619	21483	20	1509364
Caelo	Beeswax, white	14336620	22244	60	20141125
Caelo	Beeswax, white	15292022	22956	40	20150827
Caelo	Beeswax, white	20003825001	25739	50	20201123
Caelo	Beeswax, white	22000795006	26622	40	20220329
Fagron	Beeswax, white	21C26-B07-204255	25723	50	2110141
Fagron	Beeswax, white	23I12-B02-233063	27268	40	20230927
Fagron	Beeswax, white	23I12-B02-233063	27268SI	20	20230927
Bombastus	Beeswax, yellow	23002495	26910	40	20230530
Caelo	Beeswax, yellow	13335507	21433	60	20131011
Caelo	Beeswax, yellow	15317602	22245	60	20151007
Caelo	Beeswax, yellow	21004132003	26734	40	20220128
Caelo	Beeswax, yellow	21004132003	26734SI	20	20220128
Klenk	Beeswax, yellow	0290A170314	23511	40	1908177
Klenk	Beeswax, yellow	0290A170915	24870	40	20190507
Caelo	Cetyl palmitate	12331916	20865	40	1402429
Caelo	Cetyl palmitate	14351606	21875	60	20141219
Caelo	Cetyl palmitate	15301703	21984	60	AR-16-FG-007435-01
Caelo	Cetyl palmitate	15301703	22325	60	20151013
Caelo	Cetyl palmitate	160538	22486	60	20160323*
Caelo	Cetyl palmitate	17043503	23560	40	20170306
Caelo	Cetyl palmitate	171640	23639	40	20170719*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Cetyl palmitate	172715	23817	40	20171124*
Caelo	Cetyl palmitate	191390	24720	40	20190702*
Caelo	Cetyl palmitate	23001428	26959	40	20231108*
Caelo	Cocoa butter	13292013	21482	40	20130924
Caelo	Cocoa butter	14348906	22348	60	20150122
Caelo	Cocoa butter	163165	23067	40	20161116*
Caelo	Cocoa butter	17055907	23707	33	20170310
Caelo	Cocoa butter	190360	24813	40	20190227*
Caelo	Cocoa butter	19000676008	25384	40	20200318
Bombastus	Hard fat	306363	23565	34	20161213
Bombastus	Hard fat	308558	23705	40	20170321
Bombastus	Hard fat	20002467	25381	40	20200518
Caelo	Hard fat	12158122	21067	40	20120627
Caelo	Hard fat	160278	22479	60	20160407*
Caelo	Hard fat	20003131	25639	40	20201210*
Caelo	Hard fat	22002076	26362	40	20220805*
Fagron	Hard fat W35	15A07-B12-302751	21880	60	1604639
Fagron	Hard fat W35	15A07-B12-309245	22338	60	20150115
Fagron	Hard fat W35	16K08-B10-334910	23601	40	20161229
Fagron	Hard fat W35	19C04-B09-191420	25047	40	20190330
Fagron	Hard fat W35	20H17-B09-202675	25445	40	20200904
Fagron	Hard fat W35	23G27-B04-231463	27034	40	20230830
Caelo	Paraffin, hard	13390413	21731	60	20131213
Caelo	Paraffin, hard	15232004	22349	60	1702507
Caelo	Paraffin, hard	192463001	25387	40	20191024
Caelo	Paraffin, hard	21001748	26745	40	20210701
Caelo	Paraffin, hard	21001748	26745SI	20	20210701
Caelo	Paraffin, microcrystalline	14307104	21682	60	AR-15-FG-005277-01
Caelo	Paraffin, microcrystalline	14307106	21766	60	20141014
Caelo	Paraffin, microcrystalline	154128	22330	60	20160112*
Caelo	Paraffin, microcrystalline	19234501	25434	40	20191015
Caelo	Paraffin, microcrystalline	23003019	27418	40	20240126*
Caelo	Paraffin, microcrystalline	23003019	27418SI	20	20240126*
Caelo	Sodium dodecyl sulfate	13099011	20986	40	1403108
Caelo	Sodium dodecyl sulfate	15344503	22352	60	20151022
Caelo	Sodium dodecyl sulfate	16229217	23242	40	20160809
Caelo	Sodium dodecyl sulfate	170955	23278	40	20170503*
Caelo	Sodium dodecyl sulfate	191243	24715	40	20190521*
Caelo	Sodium dodecyl sulfate	190923	24716	40	20190521*
Caelo	Sodium dodecyl sulfate	20001260	25216	40	20200512*
Caelo	Sodium dodecyl sulfate	22000409	26108	40	20220427*
Caelo	Sodium dodecyl sulfate	22000409	26108SI	20	20220427*
Caelo	Sodium dodecyl sulfate	23000156	26696	40	20230209*
Caelo	Sodium dodecyl sulfate	23000156	26696SI	20	20230209*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 2847 spectra of 66 reference samples from the substance/substance group *Waxes / Fats*. These samples are listed above in the *calibration samples* section. The reference samples come from 59 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 150 115 spectra from a total of 2783 batches from further 475 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 2203 spectra of 63 reference samples from the substance/substance group *Waxes / Fats*.
- Among them are spectra of independent samples from 49 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Beeswax, white	161631	22587	40
Caelo	Beeswax, white	16163109	23513	40
Caelo	Beeswax, white	182391	24351	40
Fagron	Beeswax, white	21G17-B03-215725	26057	40
Bombastus	Beeswax, yellow	22000930	26027	40
Caelo	Beeswax, yellow	162750	22767	40
Caelo	Beeswax, yellow	17011602	23512	40
Caelo	Beeswax, yellow	20003602005	25738	50
Caelo	Beeswax, yellow	23003594	27338	40
Caelo	Cetyl palmitate	13295919	21316	20
Caelo	Cetyl palmitate	181499	24221	40
Caelo	Cetyl palmitate	182737	24356	40
Caelo	Cetyl palmitate	192859	25224	40
Caelo	Cetyl palmitate	21000860001	25933	40
Caelo	Cetyl palmitate	22000395002	26411	40
Caelo	Cetyl palmitate	24001934	27451	40
Caelo	Cocoa butter	173149	23795	40
Caelo	Cocoa butter	181351	24226	40
Caelo	Cocoa butter	182544	24363	40
Caelo	Cocoa butter	21002516002	25934	40
Caelo	Cocoa butter	23001467	27106	40
Bombastus	Hard fat	18006248	24663	40
Bombastus	Hard fat	21004219	26026	40
Bombastus	Hard fat	23001364	26623	40
Caelo	Hard fat	173076	23814	40
Caelo	Hard fat	181479	24228	40
Caelo	Hard fat	183339	24529	40
Caelo	Hard fat	191940	24887	40
Caelo	Hard fat	21003046	25846	50
Caelo	Hard fat	23000561	26700	35
Caelo	Hard fat	23001036	27120	40
Caelo	Hard fat	24001755	27450	40
Euro OTC	Hard fat	2303007	26674	40
Euro OTC	Hard fat	2307014	26920	40
Fagron	Hard fat W35	15J08-B04-324959	22806	40

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Sample ID	Spectra
Fagron	Hard fat W35	17K09-B03-343779	24114	40
Fagron	Hard fat W35	20J07-B02-202717	25748	50
Fagron	Hard fat W35	21B23-B98-211232	25908	40
Caelo	Paraffin, hard	16277704	23190	40
Caelo	Paraffin, hard	23003232	27416	40
Caelo	Paraffin, microcrystalline	15412801	23724	40
Caelo	Paraffin, microcrystalline	21003773006	26237	35
Caelo	Sodium dodecyl sulfate	13411305	21465	60
Caelo	Sodium dodecyl sulfate	16229205	23243	40
Caelo	Sodium dodecyl sulfate	172363	23664	40
Caelo	Sodium dodecyl sulfate	181822	24292	40
Caelo	Sodium dodecyl sulfate	190187	24549	40
Caelo	Sodium dodecyl sulfate	20001952	25222	40
Caelo	Sodium dodecyl sulfate	24001699	27333	40
Caelo	Beeswax, white	22000795006	26622SI†	20
Fagron	Beeswax, white	21G17-B03-215725	26057SI	10
Bombastus	Beeswax, yellow	22000930	26027SI	10
Bombastus	Beeswax, yellow	23002495	26910SI†	20
Caelo	Cetyl palmitate	13295919	21522	40
Caelo	Cetyl palmitate	21000860001	25933SI	10
Caelo	Cetyl palmitate	23001428	26959SI†	20
Caelo	Cetyl palmitate	24001934	27451SI	20
Caelo	Cocoa butter	17055907	23707†	7
Bombastus	Hard fat	306363	23565†	6
Bombastus	Hard fat	21004219	26026SI	10
Caelo	Paraffin, hard	23003232	27416SI	20
Caelo	Paraffin, microcrystalline	21003773006	26237SI	10
Caelo	Sodium dodecyl sulfate	24001699	27333SI	20

- 199 881 spectra from a total of 3991 batches from further 830 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 5726 spectra from 992 *Apo-Ident* customers from 1111 batches from the substance/substance group *Waxes / Fats*.

- Among them are spectra of independent samples from 1063 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Cocoa butter	18254412	1
	Beeswax, yellow	20000280008	1
	Beeswax, white	20000885007	1
	Hard fat	20003131003	1
	Beeswax, yellow	20003602009	1
	Cetyl palmitate	20003842013	1

continued on the next page

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

continued from previous page

Supplier	Substance	Batch	Spectra
	Beeswax, white	21001267002	1
	Beeswax, white	21001267008	1
	Beeswax, white	21001267012	2
	Beeswax, yellow	21001423003	3
	Beeswax, yellow	21001423010	3
	Paraffin, hard	2100174018	1
	Paraffin, hard	21001748004	1
	Paraffin, hard	21001748012	2
	Paraffin, hard	21001748014	3
	Paraffin, hard	21001748017	1
	Paraffin, hard	21001748018	8
	Cocoa butter	21002516020	2
	Hard fat	21003046011	1
	Beeswax, yellow	21004132003	14
	Beeswax, yellow	21004132004	4
	Beeswax, white	22000795001	6
	Beeswax, white	22000795006	4
	Beeswax, white	22000795007	8
	Cetyl palmitate	220017004	1
	Cetyl palmitate	22001717001	1
	Cetyl palmitate	22001717004	4
	Cetyl palmitate	22001785003	4
	Hard fat	22002076002	1
	Hard fat	22002076008	1
	Hard fat	22002076010	1
	Hard fat W35	22002377	1
	Cocoa butter	22003120004	4
	Cocoa butter	22003120014	1
	Beeswax, white	22003630003	6
	Beeswax, yellow	22003888002	7
	Cetyl palmitate	2201717001	1
	Hard fat W35	22J26-B12-224506	1
	Sodium dodecyl sulfate	23000156006	1
	Sodium dodecyl sulfate	23000156007	1
	Hard fat	23000447	3
	Hard fat	23000561002	16
	Hard fat	23000561003	1
	Hard fat	23000561006	1
	Hard fat	23000561008	2
	Hard fat	23001036004	1
	Paraffin, hard	23001089003	1
	Hard fat	23001364	4
	Cetyl palmitate	23001428006	11
	Cocoa butter	23001467004	2
	Cocoa butter	23001467005	3
	Beeswax, white	23002638006	1
	Paraffin, hard	23003232004	1
	Paraffin, hard	23003232005	1
	Beeswax, yellow	23003298002	1
	Hard fat	2300561002	1
	Beeswax, yellow	230120-001	1
	Beeswax, yellow	230413-001	3
	Cetyl palmitate	24000124003	1
	Beeswax, white	280A22111501	1
	Beeswax, white	280A221115-01	3
	Beeswax, white	280A230413-01	1
	Beeswax, white	280A230413-02	2
	Beeswax, yellow	290A230120-01	4
	Beeswax, yellow	290A230413-01	6
	Beeswax, yellow	30413-01	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
	Cocoa butter	423300201	1
	Beeswax, white	42374	2
	Beeswax, yellow	44064	1
/ AHD	Cocoa butter	20004174002	1
ACM	Cocoa butter	KNC1605J15	1
aep	Beeswax, yellow	21001423010	1
AHC	Beeswax, yellow	21001423003	1
AHC	Paraffin, hard	23003232005	1
AHD	Cocoa butter	14348906	1
AHD	Beeswax, yellow	15022908	1
AHD	Beeswax, yellow	18299202	1
AHD	Beeswax, white	22000795001	1
AHD	Beeswax, white	22000795006	1
AHD	Cetyl palmitate	22001785003	1
AHD	Cocoa butter	22003120004	1
AHD	Beeswax, yellow	22003888002	1
AHD	Hard fat	23000561002	1
AHD	Cetyl palmitate	23001428006	2
AHD	Beeswax, yellow	23003298002	1
AHD	Hard fat	277212	2
Alliance H.	Cetyl palmitate	15301709	1
Alliance Health 14.0…	Beeswax, yellow	280A130115	1
Alliance Healthcare	Cetyl palmitate	13131905	1
Alliance Healthcare	Beeswax, yellow	290A120627	1
Alliance Healthcare	Beeswax, white	5443200038243	1
Alliance	Paraffin, hard	21001748018	1
Alliance	Beeswax, yellow	21004132003	1
Alliance	Cetyl palmitate	22001785003	1
Alliance	Beeswax, yellow	280A130115	1
Anzag	Cocoa butter	11117816	1
Anzag	Cetyl palmitate	12018208	1
Anzag	Cocoa butter	12342004	1
Anzag	Beeswax, yellow	1462	1
Anzag	Paraffin, hard	21000732001	1
Anzag	Beeswax, yellow	23003298002	1
Anzag	Paraffin, hard	42241	1
apomix	Cocoa butter	1017300203	1
apomix	Hard fat	18147901	1
Bambastus/Gehe	Hard fat W35	18006248	1
Beiersdorf	Beeswax, white	15292014	1
BOM	Hard fat W35	22004876	1
Bombastus	Beeswax, white	16163109	1
Bombastus	Beeswax, yellow	17011604	1
Bombastus	Hard fat	17107304	2
Bombastus	Beeswax, yellow	17207405	1
Bombastus	Cocoa butter	17314901	1
Bombastus	Hard fat	18000345	1
Bombastus	Hard fat	18000346	6
Bombastus	Hard fat	18004024	6
Bombastus	Hard fat	18006248	3
Bombastus	Hard fat	19001444	1
Bombastus	Hard fat	19001445	3
Bombastus	Hard fat	19002628	1
Bombastus	Hard fat	19002629	2
Bombastus	Hard fat	20000603	7
Bombastus	Hard fat	20002467	7
Bombastus	Hard fat W35	20005051	2
Bombastus	Hard fat	21004219	2
Bombastus	Hard fat	22002377	8
Bombastus	Hard fat	22004876	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Hard fat	23000447	3
Bombastus	Beeswax, yellow	267702	1
Bombastus	Beeswax, yellow	270682	3
Bombastus	Hard fat	273759	1
Bombastus	Beeswax, yellow	279999	1
Bombastus	Beeswax, white	280A171019	1
Bombastus	Beeswax, yellow	285109	1
Bombastus	Hard fat	287287	1
Bombastus	Beeswax, yellow	290A170915	1
Bombastus	Beeswax, yellow	292025	1
Bombastus	Hard fat	293848	7
Bombastus	Beeswax, yellow	296261	1
Bombastus	Hard fat	302709	3
Bombastus	Hard fat	306363	5
Bombastus	Hard fat	308559	3
Bombastus	Beeswax, yellow	caelo	1
Bombstus/Geilenkirchen	Hard fat W35	18004024	1
cae	Beeswax, yellow	15317608	1
Cae4lo	Hard fat	15185002	1
Caele	Beeswax, yellow	17011607	1
Caelo	Beeswax, yellow		9
Caelo	Beeswax, white	10023025	1
Caelo	Cetyl palmitate	10068410	1
Caelo	Beeswax, yellow	10121302	1
Caelo	Hard fat	10158813	1
Caelo	Cocoa butter	1018302053	1
Caelo	Paraffin, hard	10194101	2
Caelo	Cocoa butter	103276705	1
Caelo	Beeswax, yellow	10364810	1
Caelo	Beeswax, yellow	10364837	1
Caelo	Beeswax, white	10651388	1
Caelo	Beeswax, yellow	11017308	1
Caelo	Beeswax, yellow	11017314	1
Caelo	Beeswax, yellow	11017315	1
Caelo	Beeswax, yellow	11017318	3
Caelo	Paraffin, hard	11021202	1
Caelo	Cetyl palmitate	11021502	1
Caelo	Cocoa butter	11034718	1
Caelo	Cocoa butter	11034719	1
Caelo	Cetyl palmitate	11042019	1
Caelo	Hard fat	11109617	1
Caelo	Hard fat	11109623	2
Caelo	Cocoa butter	11117816	1
Caelo	Sodium dodecyl sulfate	11220208	1
Caelo	Beeswax, yellow	11285001	2
Caelo	Beeswax, yellow	11285014	2
Caelo	Beeswax, yellow	11285015	1
Caelo	Beeswax, yellow	11308305	1
Caelo	Beeswax, yellow	11308311	2
Caelo	Hard fat	11345904	1
Caelo	Hard fat	11345905	3
Caelo	Hard fat	11345917	3
Caelo	Hard fat	11345918	7
Caelo	Hard fat	1135917	1
Caelo	Paraffin, hard	1136206	1
Caelo	Paraffin, hard	11363205	1
Caelo	Paraffin, hard	11363206	2
Caelo	Paraffin, hard	11363220	3
Caelo	Cetyl palmitate	12018204	3
Caelo	Cetyl palmitate	12018204/Int212191	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cetyl palmitate	12018208	6
Caelo	Cetyl palmitate	12018215	1
Caelo	Cocoa butter	12040802	1
Caelo	Cocoa butter	12040803	1
Caelo	Cocoa butter	12040807	2
Caelo	Beeswax, yellow	12041303	1
Caelo	Cetyl palmitate	12082901	1
Caelo	Beeswax, yellow	12091404	1
Caelo	Paraffin, microcrystalline	12095101	1
Caelo	Hard fat	12111204	1
Caelo	Beeswax, yellow	12124801	4
Caelo	Beeswax, yellow	12124802	2
Caelo	Beeswax, yellow	121248024-2015	1
Caelo	Beeswax, yellow	12124805	4
Caelo	Beeswax, yellow	12124806	2
Caelo	Beeswax, yellow	12124807	3
Caelo	Beeswax, yellow	12124810	4
Caelo	Beeswax, yellow	12124811	1
Caelo	Beeswax, yellow	12124812	8
Caelo	Beeswax, yellow	12124814	2
Caelo	Beeswax, yellow	12124816	1
Caelo	Beeswax, yellow	12124817	2
Caelo	Beeswax, yellow	1214816	1
Caelo	Sodium dodecyl sulfate	12153003	1
Caelo	Sodium dodecyl sulfate	12153004	1
Caelo	Sodium dodecyl sulfate	12153010	3
Caelo	Sodium dodecyl sulfate	12153019	1
Caelo	Hard fat	12158104	5
Caelo	Hard fat	12158109	3
Caelo	Hard fat	12158114	3
Caelo	Hard fat	12158115	6
Caelo	Hard fat	12158119	1
Caelo	Hard fat	12158122	1
Caelo	Cetyl palmitate	122228801/Int212191	1
Caelo	Cetyl palmitate	12228805	1
Caelo	Cetyl palmitate	12228808	3
Caelo	Cetyl palmitate	12228818	5
Caelo	Paraffin, hard	12252205	2
Caelo	Paraffin, hard	12252206	1
Caelo	Paraffin, hard	12252211	3
Caelo	Paraffin, hard	12252221	3
Caelo	Beeswax, white	122570	1
Caelo	Beeswax, yellow	12257002	3
Caelo	Beeswax, yellow	12257004	2
Caelo	Beeswax, yellow	12257009	7
Caelo	Beeswax, yellow	12257012	3
Caelo	Beeswax, yellow	12257022	3
Caelo	Cocoa butter	12270201	2
Caelo	Cocoa butter	12270202	4
Caelo	Cocoa butter	12270203	4
Caelo	Cocoa butter	12270209	2
Caelo	Cocoa butter	12270210	2
Caelo	Cetyl palmitate	1228808	1
Caelo	Beeswax, yellow	12330116	1
Caelo	Cetyl palmitate	12331916	8
Caelo	Cetyl palmitate	12331919	2
Caelo	Cocoa butter	12342003	7
Caelo	Cocoa butter	12342004	2
Caelo	Paraffin, microcrystalline	12355001	1
Caelo	Paraffin, hard	123654	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Beeswax, yellow	12367020	1
Caelo	Beeswax, yellow	12367901	12
Caelo	Beeswax, yellow	12367904	5
Caelo	Beeswax, yellow	12367910	11
Caelo	Beeswax, yellow	12367911	2
Caelo	Beeswax, yellow	12367912	3
Caelo	Beeswax, yellow	12367915	8
Caelo	Beeswax, yellow	12367916	6
Caelo	Beeswax, yellow	12367916-3429311150	1
Caelo	Beeswax, yellow	12367921	1
Caelo	Hard fat	12K01-N12	2
Caelo	Beeswax, yellow	12K20B05287421	1
Caelo	Sodium dodecyl sulfate	13014604	2
Caelo	Cocoa butter	13027202	4
Caelo	Cocoa butter	13027203	1
Caelo	Cocoa butter	13027204	4
Caelo	Cocoa butter	13027207	1
Caelo	Cocoa butter	13027221	4
Caelo	Cocoa butter	13027224	5
Caelo	Cocoa butter	13027226	4
Caelo	Cocoa butter	13027227	3
Caelo	Beeswax, yellow	13031201	4
Caelo	Beeswax, yellow	13031206	8
Caelo	Beeswax, yellow	13031220	3
Caelo	Beeswax, yellow	13031221	1
Caelo	Beeswax, yellow	13031222	3
Caelo	Beeswax, yellow	13031231	6
Caelo	Beeswax, yellow	13031239	11
Caelo	Beeswax, yellow	13051401	1
Caelo	Beeswax, yellow	13061503	1
Caelo	Sodium dodecyl sulfate	13099006	3
Caelo	Sodium dodecyl sulfate	13099011	3
Caelo	Paraffin, hard	13109203	4
Caelo	Paraffin, hard	13109213	6
Caelo	Paraffin, hard	13109214	4
Caelo	Paraffin, hard	13109218	1
Caelo	Paraffin, hard	13109221	1
Caelo	Paraffin, hard	13109224	4
Caelo	Cetyl palmitate	1313190	1
Caelo	Cetyl palmitate	13131905	3
Caelo	Cetyl palmitate	13131905NP	1
Caelo	Cetyl palmitate	13131906	8
Caelo	Cetyl palmitate	13131911	2
Caelo	Cetyl palmitate	13131914	4
Caelo	Cocoa butter	13140401	1
Caelo	Cocoa butter	13140404	2
Caelo	Cocoa butter	13140405	3
Caelo	Cocoa butter	13140406	3
Caelo	Cocoa butter	13140407	3
Caelo	Cocoa butter	13140409	1
Caelo	Hard fat	13243301	5
Caelo	Hard fat	13243403	8
Caelo	Hard fat	13243409	5
Caelo	Hard fat	13243411	3
Caelo	Hard fat	13243412	2
Caelo	Hard fat	13243414	1
Caelo	Hard fat	13243416	1
Caelo	Hard fat	13243418	3
Caelo	Hard fat	13243419	3
Caelo	Hard fat	13243420	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Paraffin, microcrystalline	13274301	1
Caelo	Paraffin, microcrystalline	13274303	5
Caelo	Cocoa butter	13292001	2
Caelo	Cocoa butter	13292006	4
Caelo	Cocoa butter	13292007	9
Caelo	Cocoa butter	13292011	2
Caelo	Cocoa butter	13292012	3
Caelo	Cocoa butter	13292013	9
Caelo	Cocoa butter	13292015	1
Caelo	Cocoa butter	13292019	3
Caelo	Cetyl palmitate	13295910	8
Caelo	Cetyl palmitate	13295919	10
Caelo	Cetyl palmitate	13295921	1
Caelo	Beeswax, yellow	133335507	1
Caelo	Beeswax, yellow	13335502	9
Caelo	Beeswax, yellow	13335503	6
Caelo	Beeswax, yellow	13335505	1
Caelo	Beeswax, yellow	13335507	6
Caelo	Beeswax, yellow	13335508	1
Caelo	Beeswax, yellow	13335509	2
Caelo	Beeswax, yellow	13335513	3
Caelo	Beeswax, yellow	13335516	1
Caelo	Beeswax, yellow	13335517	4
Caelo	Beeswax, yellow	13335518	2
Caelo	Beeswax, yellow	1335503	1
Caelo	Beeswax, yellow	13378602	1
Caelo	Beeswax, yellow	13378603	1
Caelo	Beeswax, yellow	13378619	13
Caelo	Beeswax, yellow	13378630	2
Caelo	Beeswax, yellow	13378634	6
Caelo	Beeswax, yellow	13378636	1
Caelo	Beeswax, yellow	13378639	3
Caelo	Beeswax, yellow	13378640	3
Caelo	Paraffin, hard	13390403	1
Caelo	Paraffin, hard	13390406	4
Caelo	Paraffin, hard	13390408	1
Caelo	Paraffin, hard	13390413	1
Caelo	Paraffin, hard	13390415	3
Caelo	Sodium dodecyl sulfate	13411302	2
Caelo	Sodium dodecyl sulfate	13411304	1
Caelo	Sodium dodecyl sulfate	13411305	3
Caelo	Cocoa butter	1392013	1
Caelo	Cetyl palmitate	14041505	1
Caelo	Cocoa butter	14045104	1
Caelo	Cetyl palmitate	14060705	6
Caelo	Cetyl palmitate	14060706	6
Caelo	Cetyl palmitate	14060709	6
Caelo	Cocoa butter	14123609	2
Caelo	Cocoa butter	14123611	6
Caelo	Cocoa butter	14123617	4
Caelo	Cocoa butter	14123620	6
Caelo	Cocoa butter	14123621	1
Caelo	Hard fat	1412602	1
Caelo	Hard fat	14126202	5
Caelo	Hard fat	14126203	7
Caelo	Hard fat	14126204	2
Caelo	Hard fat	14126205	1
Caelo	Hard fat	14126210	3
Caelo	Hard fat	14126216	2
Caelo	Hard fat	14126217	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hard fat	14126218	2
Caelo	Sodium dodecyl sulfate	14127406	3
Caelo	Sodium dodecyl sulfate	14127411	1
Caelo	Beeswax, yellow	1418915	1
Caelo	Beeswax, yellow	14189901	1
Caelo	Beeswax, yellow	14189902	2
Caelo	Beeswax, yellow	14189905	3
Caelo	Beeswax, yellow	14189906	1
Caelo	Beeswax, yellow	14189907	2
Caelo	Beeswax, yellow	14189908	1
Caelo	Beeswax, yellow	14189909	5
Caelo	Beeswax, yellow	14189912	6
Caelo	Beeswax, yellow	14189913	2
Caelo	Beeswax, yellow	14189914	4
Caelo	Beeswax, yellow	14189915	2
Caelo	Beeswax, yellow	14189917	3
Caelo	Beeswax, yellow	14189919	2
Caelo	Beeswax, yellow	14189920	1
Caelo	Cetyl palmitate	14213705	3
Caelo	Cetyl palmitate	14213706	1
Caelo	Cetyl palmitate	14213709	4
Caelo	Cetyl palmitate	14213710	2
Caelo	Cetyl palmitate	142137710	1
Caelo	Sodium dodecyl sulfate	14224206	1
Caelo	Sodium dodecyl sulfate	14283904	3
Caelo	Paraffin, hard	14286502	1
Caelo	Paraffin, hard	14286503	1
Caelo	Paraffin, hard	14286504	1
Caelo	Paraffin, hard	14286511	2
Caelo	Paraffin, hard	14286517	4
Caelo	Cocoa butter	14304703	1
Caelo	Paraffin, microcrystalline	14307108	2
Caelo	Paraffin, microcrystalline	14307110	1
Caelo	Beeswax, yellow	14336605	3
Caelo	Beeswax, yellow	14336607	11
Caelo	Beeswax, yellow	14336608	3
Caelo	Beeswax, yellow	14336609	2
Caelo	Beeswax, yellow	14336616	11
Caelo	Beeswax, yellow	14336617	1
Caelo	Beeswax, yellow	14336618	1
Caelo	Beeswax, yellow	14336620	8
Caelo	Beeswax, white	14336621	1
Caelo	Hard fat	14338703	3
Caelo	Hard fat	14338704	4
Caelo	Hard fat	14338705	1
Caelo	Hard fat	14338706	1
Caelo	Hard fat	14338707	3
Caelo	Hard fat	14338708	1
Caelo	Hard fat	14338711	2
Caelo	Cocoa butter	14348906	9
Caelo	Cocoa butter	14348908	2
Caelo	Cocoa butter	14348909	2
Caelo	Cetyl palmitate	14351601	2
Caelo	Cetyl palmitate	14351602	5
Caelo	Cetyl palmitate	14351606	4
Caelo	Cetyl palmitate	14351607	1
Caelo	Cetyl palmitate	14351609	3
Caelo	Cetyl palmitate	14351612	15
Caelo	Cetyl palmitate	14351614	1
Caelo	Beeswax, yellow	1436607	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Beeswax, yellow	1436616	1
Caelo	Beeswax, yellow	1436620	1
Caelo	Beeswax, yellow	14G07-B04-300495	1
Caelo	Beeswax, yellow	15022902	7
Caelo	Beeswax, yellow	15022904	4
Caelo	Beeswax, yellow	15022907	1
Caelo	Beeswax, yellow	15022908	9
Caelo	Beeswax, yellow	15023003	5
Caelo	Beeswax, yellow	15023004	9
Caelo	Beeswax, yellow	15023006	3
Caelo	Beeswax, yellow	15041301	1
Caelo	Beeswax, yellow	150622CF	1
Caelo	Cocoa butter	15088903	1
Caelo	Cocoa butter	15088904	1
Caelo	Cocoa butter	15088905	1
Caelo	Sodium dodecyl sulfate	15095404	1
Caelo	Beeswax, yellow	15098901	1
Caelo	Beeswax, yellow	15098902	1
Caelo	Hard fat	15111402	1
Caelo	Sodium dodecyl sulfate	15119907	4
Caelo	Beeswax, white	151210CA	1
Caelo	Hard fat	15185002	17
Caelo	Hard fat	15185003	11
Caelo	Hard fat	15185005	15
Caelo	Hard fat	15185007	2
Caelo	Hard fat	15185009	10
Caelo	Hard fat	1518505	1
Caelo	Paraffin, hard	1523002	1
Caelo	Paraffin, hard	152320004	1
Caelo	Paraffin, hard	15232001	1
Caelo	Paraffin, hard	15232004	8
Caelo	Cocoa butter	15246102	6
Caelo	Beeswax, white	1529003	1
Caelo	Beeswax, yellow	152920004	1
Caelo	Beeswax, white	15292002	1
Caelo	Beeswax, yellow	15292003	9
Caelo	Beeswax, yellow	15292004	14
Caelo	Beeswax, yellow	15292005	7
Caelo	Beeswax, yellow	15292007	1
Caelo	Beeswax, yellow	15292009	4
Caelo	Beeswax, white	15292010	1
Caelo	Beeswax, white	15292011	1
Caelo	Beeswax, yellow	15292014	26
Caelo	Beeswax, white	15292015	1
Caelo	Beeswax, yellow	15292022	10
Caelo	Beeswax, white	15292023	1
Caelo	Paraffin, hard	15295405	5
Caelo	Paraffin, hard	15295406	3
Caelo	Paraffin, hard	15295407	2
Caelo	Paraffin, hard	15295410	4
Caelo	Paraffin, hard	15295414	3
Caelo	Cetyl palmitate	15301701	7
Caelo	Cetyl palmitate	15301703	11
Caelo	Cetyl palmitate	15301704	6
Caelo	Cetyl palmitate	15301705	8
Caelo	Cetyl palmitate	15301708	1
Caelo	Cetyl palmitate	15301709	5
Caelo	Cetyl palmitate	15301711	7
Caelo	Beeswax, yellow	15317601	8
Caelo	Beeswax, yellow	15317602	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Beeswax, yellow	15317603	3
Caelo	Beeswax, yellow	15317607	10
Caelo	Beeswax, yellow	15317608	8
Caelo	Beeswax, yellow	15317609	12
Caelo	Beeswax, yellow	15317610	6
Caelo	Beeswax, yellow	15317611	1
Caelo	Beeswax, yellow	15317613	8
Caelo	Sodium dodecyl sulfate	15344503	5
Caelo	Sodium dodecyl sulfate	15344505	2
Caelo	Sodium dodecyl sulfate	15344510	7
Caelo	Sodium dodecyl sulfate	15344511	1
Caelo	Sodium dodecyl sulfate	15344515	2
Caelo	Paraffin, microcrystalline	15412801	2
Caelo	Paraffin, microcrystalline	15412808	1
Caelo	Cetyl palmitate	15632	1
Caelo	Beeswax, yellow	1595	1
Caelo	Paraffin, hard	16000903	3
Caelo	Paraffin, hard	16000910	2
Caelo	Paraffin, microcrystalline	16000911	5
Caelo	Paraffin, hard	16000912	5
Caelo	Paraffin, hard	16000921	4
Caelo	Paraffin, hard	16000922	3
Caelo	Hard fat	16021503	1
Caelo	Hard fat	16027801	6
Caelo	Hard fat	16027802	7
Caelo	Hard fat	16027805	4
Caelo	Hard fat	16027806	1
Caelo	Beeswax, yellow	16034206	1
Caelo	Beeswax, yellow	16038201	21
Caelo	Beeswax, yellow	16038202	19
Caelo	Beeswax, yellow	16038203	10
Caelo	Beeswax, yellow	16038205	2
Caelo	Beeswax, yellow	16038206	22
Caelo	Beeswax, yellow	16038207	10
Caelo	Beeswax, yellow	16038210	5
Caelo	Cocoa butter	16049201	4
Caelo	Cocoa butter	16049209	2
Caelo	Beeswax, yellow	16051702	1
Caelo	Cetyl palmitate	16053803	9
Caelo	Cetyl palmitate	16053804	1
Caelo	Cetyl palmitate	16053805	2
Caelo	Cetyl palmitate	16053811	8
Caelo	Cocoa butter	16062602	1
Caelo	Cocoa butter	16062604	1
Caelo	Beeswax, yellow	161202CF/15317611	1
Caelo	Beeswax, white	16163101	1
Caelo	Beeswax, white	16163105	36
Caelo	Beeswax, white	16163106	1
Caelo	Beeswax, white	16163109	21
Caelo	Beeswax, yellow	16163112	2
Caelo	Beeswax, yellow	16163114	26
Caelo	Beeswax, white	16163115	3
Caelo	Cetyl palmitate	16186805	17
Caelo	Cetyl palmitate	16186806	1
Caelo	Cetyl palmitate	16186809	18
Caelo	Sodium dodecyl sulfate	16229205	6
Caelo	Sodium dodecyl sulfate	16229206	4
Caelo	Sodium dodecyl sulfate	16229209	1
Caelo	Sodium dodecyl sulfate	16229213	2
Caelo	Sodium dodecyl sulfate	16229217	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sodium dodecyl sulfate	16229218	1
Caelo	Sodium dodecyl sulfate	16229220	3
Caelo	Hard fat W35	16271201	1
Caelo	Hard fat	16274201	15
Caelo	Hard fat	16274202	1
Caelo	Hard fat	16274203	16
Caelo	Hard fat	16274205	3
Caelo	Hard fat	16274207	1
Caelo	Hard fat	16274208	18
Caelo	Paraffin, hard	16277704	6
Caelo	Paraffin, hard	16277705	3
Caelo	Paraffin, hard	16277706	6
Caelo	Paraffin, hard	16277710	3
Caelo	Paraffin, hard	16277714	1
Caelo	Paraffin, hard	16277716	1
Caelo	Cocoa butter	163116508	1
Caelo	Cocoa butter	16315602	1
Caelo	Cocoa butter	16316501	4
Caelo	Cocoa butter	16316503	6
Caelo	Cocoa butter	16316508	26
Caelo	Cocoa butter	16316509	5
Caelo	Cocoa butter	163316508	1
Caelo	Hard fat W35	16K08-B10	1
Caelo	Paraffin, hard	17(21000732001)	1
Caelo	Beeswax, yellow	170011602	1
Caelo	Beeswax, yellow	170011607	2
Caelo	Beeswax, yellow	17011403	1
Caelo	Beeswax, yellow	17011602	14
Caelo	Beeswax, yellow	17011604	10
Caelo	Beeswax, yellow	17011605	1
Caelo	Beeswax, yellow	17011607	14
Caelo	Beeswax, yellow	17011609	9
Caelo	Beeswax, yellow	17011610	2
Caelo	Beeswax, yellow	17011611	11
Caelo	Beeswax, yellow	17011612	30
Caelo	Beeswax, yellow	17011619	1
Caelo	Beeswax, yellow	1701607	1
Caelo	Beeswax, yellow	1701611	1
Caelo	Hard fat	17041401	1
Caelo	Beeswax, yellow	17041402	1
Caelo	Cetyl palmitate	17043503	11
Caelo	Cetyl palmitate	17043504	11
Caelo	Cetyl palmitate	17043509	1
Caelo	Cocoa butter	170555901	1
Caelo	Cocoa butter	17055902	12
Caelo	Cocoa butter	17055905	1
Caelo	Cocoa butter	17055907	17
Caelo	Cocoa butter	17055908	8
Caelo	Cocoa butter	17055913	1
Caelo	Paraffin, hard	1706989	1
Caelo	Beeswax, white	17091802	37
Caelo	Beeswax, white	17091803	7
Caelo	Hard fat	170921AS/16274208	1
Caelo	Sodium dodecyl sulfate	17095504	8
Caelo	Sodium dodecyl sulfate	17095505	1
Caelo	Sodium dodecyl sulfate	17095511	13
Caelo	Hard fat	17107301	8
Caelo	Hard fat	17107304	12
Caelo	Hard fat	17107305	1
Caelo	Hard fat	17107306	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Beeswax, yellow	17121201	1
Caelo	Beeswax, yellow	17121202	1
Caelo	Paraffin, microcrystalline	17137502	1
Caelo	Cetyl palmitate	17164004	19
Caelo	Cetyl palmitate	17164005	19
Caelo	Cetyl palmitate	17164007	1
Caelo	Beeswax, yellow	172007402	1
Caelo	Beeswax, yellow	17207402	24
Caelo	Beeswax, yellow	17207403	13
Caelo	Beeswax, yellow	17207404	2
Caelo	Beeswax, yellow	17207405	1
Caelo	Sodium dodecyl sulfate	17236302	1
Caelo	Paraffin, hard	17245602	14
Caelo	Paraffin, hard	17245604	1
Caelo	Cetyl palmitate	17271502	8
Caelo	Cetyl palmitate	17271502P-180920-3	1
Caelo	Cetyl palmitate	17271502P-181227-7	1
Caelo	Cetyl palmitate	17271504	14
Caelo	Cetyl palmitate	17271505	16
Caelo	Cetyl palmitate	17271506	1
Caelo	Hard fat	17307601	37
Caelo	Hard fat	17307602	9
Caelo	Hard fat	17307603	1
Caelo	Hard fat	17307604	1
Caelo	Hard fat	17307607	2
Caelo	Hard fat	1730765	1
Caelo	Cocoa butter	17314901	4
Caelo	Cocoa butter	17314902	31
Caelo	Paraffin, hard	1734701	1
Caelo	Paraffin, hard	17347701	24
Caelo	Hard fat	18040401	17
Caelo	Hard fat	18040401P-181227-5	1
Caelo	Sodium dodecyl sulfate	18045202	2
Caelo	Sodium dodecyl sulfate	18045203	1
Caelo	Beeswax, white	18048901	46
Caelo	Beeswax, white	18048903	6
Caelo	Beeswax, white	18048904	1
Caelo	Beeswax, white	18048904P-181227-1	1
Caelo	Beeswax, yellow	18048906	40
Caelo	Beeswax, white	18048907	6
Caelo	Beeswax, yellow	18049001	29
Caelo	Beeswax, yellow	18049002	3
Caelo	Beeswax, yellow	18049003	8
Caelo	Paraffin, hard	18070103P-181227-2	1
Caelo	Paraffin, hard	18070107	30
Caelo	Paraffin, hard	18070110P-190624-3	1
Caelo	Hard fat	18070112	14
Caelo	Paraffin, hard	18070118	17
Caelo	Paraffin, hard	18070130P-200217-5	1
Caelo	Paraffin, hard	18070131	31
Caelo	Beeswax, white	180748901	1
Caelo	Beeswax, yellow	18113501	42
Caelo	Beeswax, yellow	18113502	6
Caelo	Beeswax, yellow	18113503	1
Caelo	Beeswax, yellow	18113505	47
Caelo	Beeswax, yellow	18113506	13
Caelo	Beeswax, yellow	18113507	1
Caelo	Beeswax, yellow	18113507P-191022-6	1
Caelo	Beeswax, yellow	18113507P-200102-2	1
Caelo	Beeswax, yellow	18113509	9

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Beeswax, yellow	18121201	1
Caelo	Sodium dodecyl sulfate	1812207	1
Caelo	Cocoa butter	18135101	1
Caelo	Cocoa butter	18135102	3
Caelo	Cocoa butter	18135106	4
Caelo	Cocoa butter	18135107	1
Caelo	Cocoa butter	18135112	7
Caelo	Hard fat	18147901	7
Caelo	Hard fat	18147902	32
Caelo	Hard fat	18147905	2
Caelo	Hard fat	18147907	3
Caelo	Hard fat	18147908	10
Caelo	Cetyl palmitate	181499004	1
Caelo	Cetyl palmitate	18149902	4
Caelo	Cetyl palmitate	18149904	23
Caelo	Cetyl palmitate	18149911	5
Caelo	Cetyl palmitate	18149911P-190405-3	1
Caelo	Cetyl palmitate	18149911P-190718-9	1
Caelo	Cetyl palmitate	18149912	17
Caelo	Sodium dodecyl sulfate	18182206	6
Caelo	Sodium dodecyl sulfate	18182207	1
Caelo	Sodium dodecyl sulfate	18182216	1
Caelo	Beeswax, white	18239102	34
Caelo	Beeswax, white	18239104	7
Caelo	Beeswax, white	18239106	28
Caelo	Beeswax, white	18239107	4
Caelo	Beeswax, white	18239108	1
Caelo	Beeswax, white	18239108P-191206-5	1
Caelo	Beeswax, white	18239108P-200217-4	1
Caelo	Beeswax, white	18239108P-200609-6	1
Caelo	Cocoa butter	18254402	2
Caelo	Cocoa butter	18254412	6
Caelo	Cetyl palmitate	18273704	21
Caelo	Cetyl palmitate	18273705	3
Caelo	Cetyl palmitate	18273709P-191022-5	1
Caelo	Cetyl palmitate	18273709P-200102-3	1
Caelo	Cetyl palmitate	182737704	1
Caelo	Beeswax, yellow	18299201	13
Caelo	Beeswax, yellow	18299202	7
Caelo	Beeswax, yellow	18299206	1
Caelo	Beeswax, yellow	18299208	16
Caelo	Beeswax, yellow	18299210	3
Caelo	Hard fat	18333903	1
Caelo	Hard fat	18333904	17
Caelo	Hard fat	18333905	28
Caelo	Hard fat W35	18333906	1
Caelo	Hard fat	18333908	1
Caelo	Hard fat	1833905	1
Caelo	Hard fat W35	18G13-B02-356977	1
Caelo	Cocoa butter	19000676001	1
Caelo	Cocoa butter	19000676007	2
Caelo	Cocoa butter	19000676008	4
Caelo	Cocoa butter	19000676010	1
Caelo	Cocoa butter	19000676011	5
Caelo	Sodium dodecyl sulfate	19018702	1
Caelo	Sodium dodecyl sulfate	19018704	3
Caelo	Cetyl palmitate	1902859003	1
Caelo	Beeswax, yellow	19031810	1
Caelo	Cocoa butter	190360009	5
Caelo	Cocoa butter	190360010	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Cocoa butter	19036003	5
Caelo	Cocoa butter	19036006	1
Caelo	Cocoa butter	19036007	3
Caelo	Cocoa butter	19036008	6
Caelo	Beeswax, yellow	19041704	1
Caelo	Sodium dodecyl sulfate	19075403	1
Caelo	Cetyl palmitate	190902a	1
Caelo	Sodium dodecyl sulfate	190923001	2
Caelo	Cetyl palmitate	19121803	1
Caelo	Beeswax, white	191242001	7
Caelo	Beeswax, white	191242004	21
Caelo	Beeswax, yellow	19124202	30
Caelo	Beeswax, white	19124203	2
Caelo	Beeswax, white	19124206	31
Caelo	Beeswax, white	19124207	3
Caelo	Beeswax, white	19124208	1
Caelo	Beeswax, white	19124210	21
Caelo	Beeswax, white	19124211	4
Caelo	Beeswax, yellow	191372001	29
Caelo	Beeswax, yellow	191372002	1
Caelo	Beeswax, yellow	191372003	1
Caelo	Beeswax, yellow	19137201	5
Caelo	Beeswax, yellow	19137202	35
Caelo	Beeswax, yellow	19137206	23
Caelo	Cetyl palmitate	19139004	35
Caelo	Cetyl palmitate	19139005	4
Caelo	Cetyl palmitate	19139005P-200206-4	1
Caelo	Cetyl palmitate	1913905	1
Caelo	Beeswax, yellow	1917202	1
Caelo	Hard fat	191940001	10
Caelo	Hard fat	191940002	27
Caelo	Hard fat	191940004	1
Caelo	Hard fat	191940005	8
Caelo	Hard fat	19194001	1
Caelo	Beeswax, yellow	19237202	1
Caelo	Paraffin, hard	1924603010	1
Caelo	Hard fat	192463001	24
Caelo	Paraffin, hard	192463002	1
Caelo	Paraffin, hard	192463002P-200507-7	1
Caelo	Paraffin, hard	192463009	1
Caelo	Paraffin, hard	192463010	18
Caelo	Cetyl palmitate	192859002	7
Caelo	Cetyl palmitate	192859002P-200511-2	1
Caelo	Cetyl palmitate	192859002P-200602-2	1
Caelo	Cetyl palmitate	192859003	39
Caelo	Beeswax, white	2000	1
Caelo	Beeswax, white	200000885007	1
Caelo	Hard fat	200000906007	1
Caelo	Cetyl palmitate	200000975002	1
Caelo	Beeswax, yellow	20000280002	10
Caelo	Beeswax, yellow	20000280003	17
Caelo	Beeswax, yellow	20000280005	1
Caelo	Beeswax, yellow	20000280007	4
Caelo	Beeswax, yellow	20000280008	30
Caelo	Beeswax, yellow	2000028003	1
Caelo	Beeswax, yellow	2000028007	1
Caelo	Beeswax, yellow	2000028008	1
Caelo	Hard fat W35	200003131008	1
Caelo	Beeswax, white	200003825001	1
Caelo	Cocoa butter	200004174002	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Beeswax, white	20000885003	30
Caelo	Beeswax, white	20000885004	1
Caelo	Beeswax, white	20000885007	32
Caelo	Beeswax, white	20000885008	8
Caelo	Hard fat	20000906003	14
Caelo	Hard fat	20000906004	7
Caelo	Hard fat	20000906005	2
Caelo	Hard fat	20000906007	14
Caelo	Cetyl palmitate	20000974002	6
Caelo	Cetyl palmitate	20000975002	17
Caelo	Sodium dodecyl sulfate	20001260003	2
Caelo	Cocoa butter	20001695003	14
Caelo	Cocoa butter	20001695004	2
Caelo	Beeswax, yellow	200028008	1
Caelo	Hard fat	20003131003	12
Caelo	Hard fat	20003131004	3
Caelo	Hard fat	20003131006	2
Caelo	Hard fat	20003131007	13
Caelo	Hard fat	20003131008	1
Caelo	Paraffin, hard	2000359911	1
Caelo	Beeswax, yellow	20003601001	1
Caelo	Beeswax, yellow	20003602001	18
Caelo	Beeswax, yellow	20003602002	4
Caelo	Beeswax, yellow	20003602003	5
Caelo	Beeswax, yellow	20003602005	19
Caelo	Beeswax, yellow	20003602009	7
Caelo	Beeswax, yellow	2000362001	1
Caelo	Beeswax, white	20003824003	5
Caelo	Beeswax, white	20003825001	21
Caelo	Beeswax, white	20003825005	1
Caelo	Beeswax, white	2000382501	1
Caelo	Cetyl palmitate	20003842006	5
Caelo	Cetyl palmitate	20003842013	7
Caelo	Beeswax, white	2000385001	2
Caelo	Cocoa butter	20004174002	6
Caelo	Cocoa butter	20004174003	1
Caelo	Cocoa butter	20004174009	3
Caelo	Cocoa butter	20004174010	5
Caelo	Beeswax, white	2000885008	2
Caelo	Hard fat	2000906007	1
Caelo	Cetyl palmitate	2000975002	1
Caelo	Beeswax, yellow	20031516	1
Caelo	Beeswax, yellow	20031517	1
Caelo	Hard fat	20071501	1
Caelo	Beeswax, yellow	20071503	1
Caelo	Cetyl palmitate	21000359001	15
Caelo	Cetyl palmitate	2100066001	1
Caelo	Paraffin, hard	21000732001	20
Caelo	Paraffin, hard	21000732004	1
Caelo	Paraffin, hard	21000732007	3
Caelo	Cetyl palmitate	21000860001	19
Caelo	Cetyl palmitate	21000860010	10
Caelo	Beeswax, white	21001267002	14
Caelo	Beeswax, white	21001267003	8
Caelo	Beeswax, white	21001267008	4
Caelo	Beeswax, white	21001267012	5
Caelo	Beeswax, white	21001267022	1
Caelo	Beeswax, white	2100127008	1
Caelo	Beeswax, yellow	21001423001	7
Caelo	Beeswax, yellow	21001423003	27

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Beeswax, yellow	21001423005	9
Caelo	Beeswax, yellow	21001423010	12
Caelo	Beeswax, yellow	2100143003	1
Caelo	Paraffin, hard	210017480	1
Caelo	Paraffin, hard	21001748003	1
Caelo	Paraffin, hard	21001748004	8
Caelo	Paraffin, hard	21001748007	20
Caelo	Paraffin, hard	21001748012	6
Caelo	Paraffin, hard	21001748014	2
Caelo	Sodium dodecyl sulfate	21001909003	2
Caelo	Sodium dodecyl sulfate	21001909004	1
Caelo	Cocoa butter	21002516002	12
Caelo	Cocoa butter	21002516003	3
Caelo	Cocoa butter	21002516004	6
Caelo	Cocoa butter	21002516017	3
Caelo	Cocoa butter	21002516018	1
Caelo	Cocoa butter	21002516020	5
Caelo	Cocoa butter	21002516036	1
Caelo	Hard fat	21003046008	9
Caelo	Hard fat	21003046010	2
Caelo	Hard fat	21003046011	5
Caelo	Sodium dodecyl sulfate	21003606002	1
Caelo	Paraffin, microcrystalline	21003773004	2
Caelo	Beeswax, yellow	21004132003	5
Caelo	Beeswax, yellow	21004132004	1
Caelo	Beeswax, yellow	2100423003	1
Caelo	Paraffin, hard	2100732001	1
Caelo	Cetyl palmitate	2100860001	1
Caelo	Cetyl palmitate	22000395002	8
Caelo	Beeswax, white	22000795001	4
Caelo	Beeswax, white	22000795006	10
Caelo	Cetyl palmitate	22001150003	1
Caelo	Cetyl palmitate	22001717001	1
Caelo	Cetyl palmitate	22001717004	1
Caelo	Cetyl palmitate	22001785005	1
Caelo	Hard fat	22002076002	7
Caelo	Hard fat	22002076007	2
Caelo	Hard fat	22002076011	1
Caelo	Cocoa butter	22003120014	1
Caelo	Sodium dodecyl sulfate	22003127001	2
Caelo	Beeswax, yellow	220425E	1
Caelo	Beeswax, yellow	220510/2	1
Caelo	Beeswax, yellow	22071301	1
Caelo	Beeswax, yellow	220829C	1
Caelo	Beeswax, white	2271200	1
Caelo	Hard fat	23000561002	2
Caelo	Hard fat	24011302	1
Caelo	Sodium dodecyl sulfate	26031508	1
Caelo	Cetyl palmitate	26071201	1
Caelo	Beeswax, yellow	26091302	1
Caelo	Hard fat	27101703	1
Caelo	Beeswax, yellow	280003	1
Caelo	Beeswax, yellow	28011501	1
Caelo	Cetyl palmitate	28041731	1
Caelo	Beeswax, white	280A150528	1
Caelo	Beeswax, white	280A171019	1
Caelo	Beeswax, white	280A220609-02	1
Caelo	Hard fat	29061803	1
Caelo	Beeswax, white	29091805	1
Caelo	Beeswax, yellow	290A0151214	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Beeswax, yellow	290A170915	4
Caelo	Hard fat	293848	1
Caelo	Beeswax, yellow	30011407	1
Caelo	Paraffin, microcrystalline	30101202	1
Caelo	Cetyl palmitate	30101301	1
Caelo	Beeswax, yellow	30101308	1
Caelo	Paraffin, hard	302709	1
Caelo	Paraffin, microcrystalline	3042012M1	1
Caelo	Beeswax, white	3051808	1
Caelo	Beeswax, yellow	3253	1
Caelo	Cetyl palmitate	3785734	1
Caelo	Beeswax, yellow	4031403	1
Caelo	Cetyl palmitate	43204210008601	1
Caelo	Beeswax, yellow	4910A-01239	1
Caelo	Beeswax, yellow	5022904	1
Caelo	Beeswax, yellow	5121707	1
Caelo	Cocoa butter	515A-03176	1
Caelo	Paraffin, microcrystalline	52622395	1
Caelo	Beeswax, yellow	61(20003602001)	1
Caelo	Beeswax, yellow	6111407	1
Caelo	Beeswax, yellow	7091704	1
Caelo	Hard fat	7101304	1
Caelo	Paraffin, microcrystalline	7111201	1
Caelo	Paraffin, microcrystalline	7111202	1
Caelo	Sodium dodecyl sulfate	720E-01907	1
Caelo	Hard fat	8041710	1
Caelo	Hard fat	8051810	1
Caelo	Hard fat	90915429	1
Caelo	Hard fat W35	W0000906005	2
Caesa / Alliance Hea…	Beeswax, white	20003825001	1
Caesa / Alliance Hea…	Cetyl palmitate	20003842013	1
Caesar & Lorenz GmbH	Cetyl palmitate	17043504	1
Caesar & Lorenz GmbH	Cetyl palmitate	18149912	1
Caesar & Lorenz GmbH	Sodium dodecyl sulfate	18182206	1
Caesar & Lorenz GmbH	Sodium dodecyl sulfate	19018704	1
Caesar & Lorenz GmbH	Cetyl palmitate	19139004	2
Caesar & Lorenz GmbH	Cetyl palmitate	192859003	1
Caesar & Lorenz	Cocoa butter	13140404	1
Caesar & Lorenz	Beeswax, white	20003824003	1
Caesar & Loretz GmbH…	Paraffin, hard	21001748007	1
Caesar & Loretz GmbH…	Beeswax, yellow	15023004	1
Caesar & Loretz GmbH…	Beeswax, white	15292010	1
Caesar & Loretz GmbH…	Cocoa butter	16316503	1
Caesar & Loretz GmbH…	Cocoa butter	17055908	1
Caesar & Loretz GmbH…	Beeswax, white	20000885007	1
Caesar & Loretz GmbH…	Hard fat	191940002	1
Caesar & Loretz GmbH…	Hard fat	191940005	3
Caesar & Loretz GmbH…	Beeswax, white	19124210	1
Caesar & Loretz GmbH…	Cetyl palmitate	192859003	1
Caesar & Loretz GmbH…	Beeswax, yellow	15317613	1
Caesar & Loretz GmbH…	Beeswax, white	16163115	3
Caesar & Loretz GmbH…	Sodium dodecyl sulfate	16229205	1
Caesar & Loretz GmbH…	Cocoa butter	16316509	1
Caesar & Loretz GmbH…	Cetyl palmitate	17271505	1
Caesar & Loretz GmbH…	Beeswax, white	18048907	2
Caesar & Loretz GmbH…	Beeswax, yellow	18049001	1
Caesar & Loretz GmbH…	Beeswax, yellow	18113505	1
Caesar & Loretz GmbH…	Cocoa butter	190360009	1
Caesar & Loretz GmbH…	Hard fat	20000906003	1
Caesar & Loretz GmbH…	Hard fat	20003131003	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Beeswax, yellow	21001423001	1
Caesar & Loretz GmbH...	Beeswax, yellow	21004132003	1
Caesar & Loretz GmbH...	Cetyl palmitate	22000395002	1
Caesar & Loretz GmbH...	Cetyl palmitate	22001785003	1
Caesar & Loretz GmbH...	Cetyl palmitate	18149912	1
Caesar & Loretz GmbH...	Beeswax, white	20000280008	2
Caesar & Loretz GmbH...	Paraffin, hard	18070118	1
Caesar & Loretz GmbH...	Beeswax, yellow	18113509	1
Caesar & Loretz GmbH...	Cetyl palmitate	19139004	1
Caesar & Loretz GmbH...	Cetyl palmitate	192859003	1
Caesar & Loretz GmbH...	Hard fat	17307607	1
Caesar & Loretz GmbH...	Hard fat	12158104	1
Caesar & Loretz GmbH...	Beeswax, yellow	11285008	1
Caesar & Loretz GmbH...	Hard fat	11345918	1
Caesar & Loretz GmbH...	Beeswax, yellow	12367901	1
Caesar & Loretz GmbH...	Beeswax, yellow	12367910	1
Caesar & Loretz GmbH...	Hard fat	13243403	1
Caesar & Loretz GmbH...	Beeswax, yellow	18113505	1
Caesar & Loretz GmbH...	Beeswax, yellow	18049001	1
Caesar & Loretz GmbH...	Hard fat	18333905	2
Caesar & Loretz GmbH...	Hard fat	18147908	1
Caesar & Loretz GmbH...	Hard fat	18333904	1
Caesar & Loretz GmbH...	Paraffin, hard	192463010	1
Caesar & Loretz GmbH...	Cocoa butter	21002516002	1
Caesar & Loretz GmbH...	Beeswax, yellow	20000280003	1
Caesar & Loretz GmbH...	Cocoa butter	18254412	1
Caesar & Loretz GmbH...	Beeswax, yellow	191372001	1
Caesar & Loretz GmbH...	Paraffin, hard	21000732001	1
Caesar & Loretz GmbH/ Ph	Beeswax, yellow	18299201	1
Caesar & Loretz GmbH...	Beeswax, yellow	21001423001	2
Caesar & Loretz GmbH...	Hard fat	20003131008	2
Caesar & Loretz GmbH/AHD	Beeswax, yellow	19137206	1
Caesar & Loretz GmbH/AHD	Beeswax, white	20003825001	2
Caesar & Loretz GmbH/AHD	Cocoa butter	20004174009	2
Caesar & Loretz GmbH...	Beeswax, yellow	20003602005	1
Caesar & Loretz GmbH...	Cocoa butter	20004174002	1
Caesar & Loretz GmbH...	Hard fat	18147908	1
Caesar & Loretz GmbH...	Hard fat	18333905	2
Caesar & Loretz GmbH...	Beeswax, white	20000885003	1
Caesar & Loretz GmbH/E	Hard fat	18333904	1
Caesar & Loretz GmbH/E	Beeswax, white	20000885003	1
Caesar & Loretz GmbH/E	Beeswax, yellow	20003602001	1
Caesar & Loretz GmbH...	Cocoa butter	18254402	1
Caesar & Loretz GmbH...	Hard fat	18333904	1
Caesar & Loretz GmbH...	Hard fat	18333905	1
Caesar & Loretz GmbH...	Hard fat	191940002	1
Caesar & Loretz GmbH...	Hard fat	20000906003	1
Caesar & Loretz GmbH...	Cetyl palmitate	20000975002	1
Caesar & Loretz GmbH...	Cetyl palmitate	21000359001	1
Caesar & Loretz GmbH/Gehe	Cocoa butter	19036003	1
Caesar & Loretz GmbH/Gehe	Beeswax, white	19124206	1
Caesar & Loretz GmbH/Gehe	Beeswax, yellow	191372001	2
Caesar & Loretz GmbH/GEHE	Beeswax, yellow	19137202	1
Caesar & Loretz GmbH/Gehe	Cetyl palmitate	192859003	3
Caesar & Loretz GmbH/Gehe	Hard fat	20003131007	2
Caesar & Loretz GmbH/Gehe	Cetyl palmitate	20003842013	1
Caesar & Loretz GmbH...	Hard fat	18147908	1
Caesar & Loretz GmbH...	Beeswax, white	19124206	1
Caesar & Loretz GmbH...	Beeswax, white	20000885008	2
Caesar & Loretz GmbH...	Cetyl palmitate	21000359001	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH...	Cetyl palmitate	21000860010	1
Caesar & Loretz GmbH...	Cocoa butter	22003120004	1
Caesar & Loretz GmbH/K	Beeswax, yellow	18113505	1
Caesar & Loretz GmbH/Kehr	Beeswax, white	21001267012	2
Caesar & Loretz GmbH...	Beeswax, yellow	19137202	3
Caesar & Loretz GmbH...	Beeswax, yellow	19137202	1
Caesar & Loretz GmbH...	Beeswax, yellow	19137206	1
Caesar & Loretz GmbH...	Beeswax, yellow	20000280003	1
Caesar & Loretz GmbH...	Beeswax, yellow	20000280007	1
Caesar & Loretz GmbH...	Hard fat	20003131003	1
Caesar & Loretz GmbH...	Beeswax, yellow	20003602005	1
Caesar & Loretz GmbH...	Beeswax, yellow	21001423003	1
Caesar & Loretz GmbH/PH	Cetyl palmitate	18273704	1
Caesar & Loretz GmbH/Ph	Beeswax, yellow	191372001	1
Caesar & Loretz GmbH/Ph	Cetyl palmitate	192859003	1
Caesar & Loretz GmbH/Ph	Beeswax, yellow	2000080008	1
Caesar & Loretz GmbH...	Beeswax, yellow	20003602009	1
Caesar & Loretz GmbH...	Beeswax, white	21001267003	2
Caesar & Loretz GmbH...	Beeswax, white	21001267008	1
Caesar & Loretz GmbH...	Beeswax, yellow	21001423010	1
Caesar & Loretz GmbH...	Paraffin, hard	21001748007	1
Caesar & Loretz GmbH...	Paraffin, hard	21001748012	1
Caesar & Loretz GmbH...	Beeswax, yellow	191372001	1
Caesar & Loretz GmbH...	Hard fat	18333904	2
Caesar & Loretz GmbH...	Beeswax, yellow	19137202	1
Caesar & Loretz GmbH...	Cetyl palmitate	192859003	1
Caesar & Loretz GmbH...	Cetyl palmitate	20000974002	1
Caesar & Loretz GmbH...	Beeswax, yellow	20003602001	1
Caesar & Loretz GmbH...	Hard fat	21003046011	2
Caesar & Loretz GmbH...	Cetyl palmitate	220001717001	1
Caesar & Loretz GmbH...	Cetyl palmitate	22001717001	1
Caesar & Loretz GmbH...	Hard fat	22002076002	1
Caesar & Loretz GmbH...	Hard fat	22002076008	1
Caesar & Loretz GmbH/Sa	Beeswax, white	19124206	2
Caesar & Loretz GmbH/Sa	Cetyl palmitate	20000974002	1
Caesar & Loretz GmbH/Sa	Cetyl palmitate	20000975002	1
Caesar & Loretz GmbH...	Beeswax, yellow	18113507	1
Caesar & Loretz GmbH...	Cetyl palmitate	18273704	1
Caesar & Loretz GmbH...	Beeswax, yellow	18299210	1
Caesar & Loretz GmbH...	Hard fat	183339	1
Caesar & Loretz GmbH...	Hard fat	18333906	1
Caesar & Loretz GmbH...	Beeswax, white	191242001	1
Caesar & Loretz GmbH...	Beeswax, yellow	19137203	1
Caesar & Loretz GmbH...	Hard fat	19194001	1
Caesar & Loretz GmbH...	Cetyl palmitate	192859003	3
Caesar & Loretz GmbH...	Beeswax, yellow	20000280007	1
Caesar & Loretz GmbH...	Beeswax, yellow	2000028005	1
Caesar & Loretz GmbH...	Beeswax, white	20000885008	2
Caesar & Loretz GmbH...	Cetyl palmitate	20000974002	1
Caesar & Loretz GmbH...	Beeswax, white	20003825001	1
Caesar & Loretz GmbH...	Cetyl palmitate	21000860009	1
Caesar & Loretz GmbH...	Beeswax, yellow	21001423005	1
Caesar & Loretz GmbH...	Sodium dodecyl sulfate	21001909003	1
Caesar & Loretz GmbH...	Hard fat	21003046008	1
Caesar & Loretz GmbH...	Cetyl palmitate	22000395002	1
Caesar & Loretz GmbH...	Beeswax, white	22000795001	1
Caesar & Loretz GmbH...	Hard fat	22002076001	1
Caesar & Loretz GmbH...	Beeswax, yellow	18113502	1
Caesar & Loretz GmbH	Cetyl palmitate	10068402	2
Caesar & Loretz GmbH	Cocoa butter	12270210	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Beeswax, yellow	12367910	1
Caesar & Loretz GmbH	Beeswax, yellow	13031221	1
Caesar & Loretz GmbH	Beeswax, white	16163105	1
Caesar & Loretz GmbH	Cetyl palmitate	16186805	1
Caesar & Loretz GmbH	Sodium dodecyl sulfate	17095504	1
Caesar & Loretz GmbH	Cetyl palmitate	17164005	1
Caesar & Loretz GmbH	Hard fat W35	17307601	1
Caesar & Loretz GmbH	Paraffin, hard	17347701	1
Caesar & Loretz GmbH	Hard fat	18040401	1
Caesar & Loretz GmbH	Beeswax, white	18048901	1
Caesar & Loretz GmbH	Beeswax, white	18048906	2
Caesar & Loretz GmbH	Paraffin, hard	18070107	4
Caesar & Loretz GmbH	Paraffin, hard	18070110	1
Caesar & Loretz GmbH	Paraffin, hard	18070112	1
Caesar & Loretz GmbH	Paraffin, hard	18070118	3
Caesar & Loretz GmbH	Paraffin, hard	18070130	1
Caesar & Loretz GmbH	Paraffin, hard	18070131	4
Caesar & Loretz GmbH	Beeswax, yellow	18113502	1
Caesar & Loretz GmbH	Beeswax, yellow	18113505	3
Caesar & Loretz GmbH	Beeswax, yellow	18113506	1
Caesar & Loretz GmbH	Beeswax, yellow	18113509	1
Caesar & Loretz GmbH	Cocoa butter	18135106	2
Caesar & Loretz GmbH	Hard fat	18147902	2
Caesar & Loretz GmbH	Hard fat	18147908	1
Caesar & Loretz GmbH	Cetyl palmitate	18149904	2
Caesar & Loretz GmbH	Cetyl palmitate	18149911	1
Caesar & Loretz GmbH	Cetyl palmitate	18149912	1
Caesar & Loretz GmbH	Sodium dodecyl sulfate	18182206	1
Caesar & Loretz GmbH	Beeswax, white	18239102	7
Caesar & Loretz GmbH	Beeswax, white	18239104	5
Caesar & Loretz GmbH	Beeswax, white	18239106	4
Caesar & Loretz GmbH	Beeswax, white	18239107	2
Caesar & Loretz GmbH	Cocoa butter	18254402	2
Caesar & Loretz GmbH	Cetyl palmitate	18273704	10
Caesar & Loretz GmbH	Cetyl palmitate	18273705	1
Caesar & Loretz GmbH	Cetyl palmitate	18273709	2
Caesar & Loretz GmbH	Beeswax, yellow	18299201	1
Caesar & Loretz GmbH	Beeswax, yellow	18299202	2
Caesar & Loretz GmbH	Beeswax, yellow	18299203	1
Caesar & Loretz GmbH	Beeswax, yellow	18299206	2
Caesar & Loretz GmbH	Beeswax, yellow	18299210	1
Caesar & Loretz GmbH	Hard fat	18333903	2
Caesar & Loretz GmbH	Hard fat	18333904	3
Caesar & Loretz GmbH	Hard fat	18333905	9
Caesar & Loretz GmbH	Cocoa butter	19000676011	1
CAESAR & LORETZ GMBH	Cocoa butter	190360009	1
Caesar & Loretz GmbH	Cocoa butter	19036007	2
Caesar & Loretz GmbH	Cocoa butter	19036008	3
Caesar & Loretz GmbH	Cocoa butter	19036011	3
Caesar & Loretz GmbH	Sodium dodecyl sulfate	19075403	1
Caesar & Loretz GmbH	Beeswax, white	191242004	1
Caesar & Loretz GmbH	Beeswax, white	19124202	6
Caesar & Loretz GmbH	Beeswax, white	19124203	5
Caesar & Loretz GmbH	Beeswax, white	19124206	5
Caesar & Loretz GmbH	Beeswax, white	19124210	4
Caesar & Loretz GmbH	Beeswax, white	19124211	4
Caesar & Loretz GmbH	Beeswax, yellow	19137202	9
Caesar & Loretz GmbH	Beeswax, yellow	19137203	1
Caesar & Loretz GmbH	Beeswax, yellow	19137206	2
Caesar & Loretz GmbH	Cetyl palmitate	19139004	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Cetyl palmitate	19139005	1
Caesar & Loretz GmbH	Beeswax, yellow	19172001	1
Caesar & Loretz GmbH	Hard fat	191940001	3
Caesar & Loretz GmbH	Hard fat	191940002	11
Caesar & Loretz GmbH	Hard fat	19194001	1
Caesar & Loretz GmbH	Paraffin, hard	192463001	8
Caesar & Loretz GmbH	Paraffin, hard	192463010	2
Caesar & Loretz GmbH	Cetyl palmitate	192859002	4
Caesar & Loretz GmbH	Cetyl palmitate	192859003	18
Caesar & Loretz GmbH	Beeswax, yellow	20000280002	5
CAESAR & LORETZ GMBH	Beeswax, yellow	20000280003	1
Caesar & Loretz GmbH	Beeswax, yellow	20000280007	3
Caesar & Loretz GmbH	Beeswax, yellow	20000280008	5
Caesar & Loretz GmbH	Beeswax, white	20000885003	6
Caesar & Loretz GmbH	Beeswax, white	20000885004	2
Caesar & Loretz GmbH	Beeswax, white	20000885007	13
Caesar & Loretz GmbH	Beeswax, white	20000885008	1
Caesar & Loretz GmbH	Hard fat	20000906003	5
CAESAR & LORETZ GMBH	Hard fat	20000906003	2
Caesar & Loretz GmbH	Hard fat	20000906004	4
Caesar & Loretz GmbH	Hard fat	20000906005	2
Caesar & Loretz GmbH	Hard fat	20000906007	4
Caesar & Loretz GmbH	Hard fat	20000906008	2
Caesar & Loretz GmbH	Cetyl palmitate	20000974002	2
Caesar & Loretz GmbH	Cetyl palmitate	20000975002	5
Caesar & Loretz GmbH	Sodium dodecyl sulfate	20001260003	1
Caesar & Loretz GmbH	Cocoa butter	20001695002	2
Caesar & Loretz GmbH	Cocoa butter	20001695003	5
Caesar & Loretz GmbH	Beeswax, yellow	20001776002	2
Caesar & Loretz GmbH	Hard fat	20003131003	4
Caesar & Loretz GmbH	Hard fat	20003131004	2
Caesar & Loretz GmbH	Hard fat	20003131007	2
Caesar & Loretz GmbH	Hard fat	20003131008	3
Caesar & Loretz GmbH	Beeswax, yellow	20003602001	8
Caesar & Loretz GmbH	Beeswax, yellow	20003602002	4
Caesar & Loretz GmbH	Beeswax, yellow	20003602003	2
Caesar & Loretz GmbH	Beeswax, yellow	20003602005	6
Caesar & Loretz GmbH	Beeswax, yellow	20003602009	3
CAESAR & LORETZ GMBH	Beeswax, yellow	20003602009	1
Caesar & Loretz GmbH	Beeswax, white	20003824003	2
Caesar & Loretz GmbH	Beeswax, yellow	20003825001	10
Caesar & Loretz GmbH	Cetyl palmitate	20003842006	1
Caesar & Loretz GmbH	Cetyl palmitate	20003842013	4
Caesar & Loretz GmbH	Cocoa butter	20004174002	2
Caesar & Loretz GmbH	Cocoa butter	20004174006	4
Caesar & Loretz GmbH	Cocoa butter	20004174010	2
Caesar & Loretz GmbH	Cetyl palmitate	21000359001	11
Caesar & Loretz GmbH	Paraffin, hard	21000732001	10
Caesar & Loretz GmbH	Cetyl palmitate	21000860001	5
Caesar & Loretz GmbH	Cetyl palmitate	21000860009	3
Caesar & Loretz GmbH	Cetyl palmitate	21000860010	12
Caesar & Loretz GmbH	Beeswax, white	21001267002	2
CAESAR & LORETZ GMBH	Beeswax, white	21001267002	1
Caesar & Loretz GmbH	Beeswax, white	21001267008	4
Caesar & Loretz GmbH	Beeswax, white	21001267012	2
Caesar & Loretz GmbH	Beeswax, yellow	21001423001	2
Caesar & Loretz GmbH	Beeswax, yellow	21001423003	4
Caesar & Loretz GmbH	Beeswax, yellow	21001423004	5
Caesar & Loretz GmbH	Beeswax, yellow	21001423010	2
Caesar & Loretz GmbH	Paraffin, hard	21001748004	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Paraffin, hard	21001748007	3
Caesar & Loretz GmbH	Paraffin, hard	21001748014	1
Caesar & Loretz GmbH	Cocoa butter	21002516002	3
Caesar & Loretz GmbH	Cocoa butter	21002516004	2
Caesar & Loretz GmbH	Cocoa butter	21002516017	1
Caesar & Loretz GmbH	Cocoa butter	21002516018	1
Caesar & Loretz GmbH	Cocoa butter	21002516020	2
Caesar & Loretz GmbH	Hard fat	21003046001	2
Caesar & Loretz GmbH	Hard fat	21003046008	14
Caesar & Loretz GmbH	Hard fat	21003046009	2
Caesar & Loretz GmbH	Hard fat	21003046011	5
Caesar & Loretz GmbH	Paraffin, microcrystalline	21003773003	1
Caesar & Loretz GmbH	Beeswax, yellow	21004132003	4
Caesar & Loretz GmbH	Cetyl palmitate	22000395002	3
Caesar & Loretz GmbH	Beeswax, white	22000795006	2
Caesar & Loretz GmbH	Cetyl palmitate	22001717004	1
Caesar & Loretz GmbH	Hard fat	22002076002	1
Caesar & Loretz GmbH	Hard fat	22002076007	1
Caesar & Loretz GmbH	Hard fat	22002076010	3
Caesar & Loretz GmbH	Sodium dodecyl sulfate	22003127001	1
Caesar & Loretz GmbH	Beeswax, white	2200795006	1
Caesar & Loretz GmbH	Sodium dodecyl sulfate	23000156006	1
Caesar & Loretz GmbH...	Cetyl palmitate	20000975002	1
Caesar & Loretz Hild...	Hard fat	20000906003	1
Caesar & Loretz Hild...	Beeswax, yellow	19137202	1
Caesar & Loretz/AHD	Beeswax, yellow	16038206	1
Caesar & Loretz/Gehe	Beeswax, yellow	191372001	1
Caesar & Loretz/Gehe	Beeswax, yellow	19137202	1
Caesar & Loretz/Geil...	Beeswax, yellow	19137202	2
Caesar & Loretz/Noweda	Beeswax, white	191242001	1
Caesar & Loretz/Noweda	Beeswax, white	19124210	1
Caesar & Loretz/Noweda	Paraffin, hard	192463001	1
Caesar & Loretz/Noweda	Beeswax, white	20000885004	1
Caesar & Loretz	Beeswax, yellow	15317613	1
Caesar & Loretz	Beeswax, yellow	16038201	1
Caesar & Loretz	Paraffin, hard	18070107	1
Caesar / Ebert	Paraffin, hard	15295405	1
Caesar / Gehe	Beeswax, yellow	15023004	1
Caesar / Gehe	Beeswax, yellow	15292009	1
Caesar Loretz Gmbh	Hard fat	17307602	1
Caesar u Loretz	Cetyl palmitate	14213710	1
Caesar und Loretz GmbH	Hard fat	18040401	1
Caesar&Lorenz	Beeswax, yellow	21001423001	1
Caesar&Loretz GmbH D...	Hard fat	11109617	1
Caesar&Loretz GmbH	Beeswax, yellow	16038210	1
Caesar&Loretz	Cetyl palmitate	17271504	2
Caesar/Gehe	Beeswax, white	18048906	1
Caesar/Noweda	Beeswax, yellow	12124811	3
Caesar/Noweda	Cetyl palmitate	12228801	1
Caesar/Noweda	Beeswax, yellow	13031220	1
Caesar/Noweda	Cetyl palmitate	13295909	1
Caesar/Noweda	Hard fat	14126203	1
Caesar/Noweda	Cetyl palmitate	15301701	1
Caeser und Loretz GmbH	Hard fat	18333905	1
Caleo/ Noweda	Beeswax, yellow	18049003	1
Caleo/Sanacorp	Beeswax, yellow	18299201	1
calo	Beeswax, yellow	17011612	1
Carlo/Gehe/10,80	Cetyl palmitate	18273705	1
Carlo/Gehe/8,52	Beeswax, yellow	18299206	1
Cealo / Noweda	Cocoa butter	13292011	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Cealo / Anzag	Paraffin, hard	220826(21001748007)	1
Cealo/AHD	Paraffin, hard	15295411	2
Cealo/Gehe	Beeswax, yellow	13335502	1
Cealo/GEHE	Cetyl palmitate	192859003	1
Cealo/Kehr	Beeswax, yellow	20000280002	1
Cealo/Noweda	Cetyl palmitate	22000395002	1
Cealo/Phoenix	Cetyl palmitate	20003842006	4
Cealo/Sanacorp	Hard fat	20003131007	1
Cealo	Beeswax, yellow	18113509	1
Cealo	Paraffin, hard	21000732007	1
Cealo	Cetyl palmitate	21000860001	1
Ceasar & Loretz GmbH…	Cetyl palmitate	18149904	1
Cesar&Loretz GmbH Noweda	Cetyl palmitate	20000974002	1
China Medica	Hard fat	3244303	1
coelo/Sana	Cetyl palmitate	14351612	1
Cordes/Gehe	Beeswax, white	18048907	1
E Plus	Beeswax, yellow	17011612	3
Ebert + Jacobi	Hard fat W35	20000603	3
E-Plus	Beeswax, yellow	16038202	1
Euro OTC	Beeswax, yellow	1201012-01	1
Euro OTC	Cetyl palmitate	12228808	1
Euro OTC	Paraffin, hard	13109224	1
Euro OTC	Beeswax, yellow	1407013-01	1
Euro OTC	Cocoa butter	14123621	1
Euro OTC	Beeswax, yellow	1503013-01	1
Euro OTC	Hard fat	15185005	1
Euro OTC	Paraffin, hard	15232004	1
Euro OTC	Cetyl palmitate	15301705	1
Euro OTC	Beeswax, yellow	16038201	1
Euro OTC	Cetyl palmitate	160419C	1
Euro OTC	Beeswax, white	16163104	1
Euro OTC	Cetyl palmitate	16186809	1
Euro OTC	Cocoa butter	16316508	1
Euro OTC	Beeswax, yellow	17011607	1
Euro OTC	Beeswax, white	17091802	1
Euro OTC	Hard fat	17107304	1
Euro OTC	Hard fat W35	17K09B03343780	1
Euro OTC	Hard fat	18004023	1
Euro OTC	Paraffin, hard	18070107	1
Euro OTC	Beeswax, yellow	18113501	1
Euro OTC	Beeswax, yellow	18113505	3
Euro OTC	Cetyl palmitate	18149904	1
Euro OTC	Cetyl palmitate	19139005	2
Euro OTC	Cetyl palmitate	20000975002	1
Euro OTC	Cetyl palmitate	20003842013	1
Euro/Sanacorp	Beeswax, yellow	1708506	1
Euroo	Beeswax, yellow	1407013-01	1
Fagron	Hard fat		1
Fagron	Hard fat	12158115	2
Fagron	Cetyl palmitate	12C27-N07	2
Fagron	Cetyl palmitate	12D19-N02	1
Fagron	Beeswax, yellow	12D23-N05	2
Fagron	Hard fat	12G04-N18	1
Fagron	Hard fat	12I04-N11	1
Fagron	Hard fat	12K01-N12	1
Fagron	Hard fat	13243301	1
Fagron	Beeswax, yellow	13B04-N04	2
Fagron	Hard fat	13D10-N06	1
Fagron	Beeswax, yellow	13I02-B01	1
Fagron	Beeswax, yellow	13L02-B01-291452	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Beeswax, yellow	13L02-B01-294113	2
Fagron	Beeswax, yellow	13L02-B01-294114	1
Fagron	Beeswax, yellow	14336616	1
Fagron	Hard fat	14G03-B03-296731	1
Fagron	Beeswax, yellow	14G07-B04-300495	3
Fagron	Hard fat	14L01-B06	2
Fagron	Hard fat	14L01-B06-303380	3
Fagron	Beeswax, white	15292009	1
Fagron	Beeswax, white	15292022	1
Fagron	Beeswax, yellow	15317603	1
Fagron	Hard fat W35	15A07-B12-309245	1
Fagron	Hard fat	15F03-B06	4
Fagron	Hard fat	15F03-B06-308708	3
Fagron	Hard fat W35	15J08-B04-322726	1
Fagron	Hard fat W35	15J08-B04-322727	1
Fagron	Hard fat W35	15J08-B04-324217	1
Fagron	Hard fat W35	15J08-B04-324959	2
Fagron	Sodium dodecyl sulfate	16229205	1
Fagron	Beeswax, white	16a28_b10_322948	1
Fagron	Beeswax, white	16A28-B10-322948	1
Fagron	Hard fat	16H01-B03-334976	2
Fagron	Beeswax, white	16J28-B06	1
Fagron	Hard fat W35	16K08-B10-328956	1
Fagron	Hard fat W35	16K08-B10-332763	3
Fagron	Hard fat W35	16k08-b10-334910	1
Fagron	Hard fat W35	16K08-B10-339077	6
Fagron	Hard fat W35	16K09-B03-346709	1
Fagron	Hard fat W35	16K-B10-334910	1
Fagron	Beeswax, yellow	17011607	1
Fagron	Beeswax, white	1701947	1
Fagron	Beeswax, white	17091802	1
Fagron	Cetyl palmitate	17164005	1
Fagron	Paraffin, hard	17245604	1
Fagron	Beeswax, white	17C15-B01-342088	1
Fagron	Beeswax, white	17C15-B01-354806	1
Fagron	Hard fat W35	17K09-B03	2
Fagron	Hard fat W35	17k09-b03-346709	1
Fagron	Hard fat W35	17K09-B03-346709	5
Fagron	Hard fat W35	17K09-B03-348770	4
Fagron	Hard fat W35	17k09-b03-351980	1
Fagron	Hard fat W35	17K09-B03-351980	5
Fagron	Hard fat W35	17K09-B03-355397	1
Fagron	Beeswax, white	17L04-B05-348865	3
Fagron	Cetyl palmitate	18149904	1
Fagron	Sodium dodecyl sulfate	18182206	1
Fagron	Hard fat W35	18G13-B02	1
Fagron	Hard fat W35	18G13-B02-355398	1
Fagron	Hard fat W35	18G13-B02-356977	4
Fagron	Hard fat W35	18G13B02356978	1
Fagron	Hard fat	18I12-B04-354348	1
Fagron	Hard fat W35	19C04-B04	1
Fagron	Hard fat W35	19C04-B09	2
Fagron	Hard fat W35	19C04-B09-191420	2
Fagron	Hard fat W35	19C04B09191422	1
Fagron	Hard fat W35	19CO4-B04	1
Fagron	Hard fat	19I09-F04	2
Fagron	Hard fat	19I09-F04-365037	3
Fagron	Beeswax, white	19J17-B01-196942	2
Fagron	Hard fat W35	20A08-B03	1
Fagron	Hard fat	20A08-B03-197663	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Hard fat W35	20A08-B03-197664	3
Fagron	Hard fat W35	20A08-B03-197665	1
Fagron	Cetyl palmitate	20B04-F08	1
Fagron	Hard fat	20B04-F08-368439	1
Fagron	Hard fat W35	20F10-B05	1
Fagron	Hard fat	20F10-B05-201350	2
Fagron	Hard fat W35	20G01-F02	1
Fagron	Hard fat	20G01-F02-372412	2
Fagron	Hard fat	20G01-F02-372412210030	1
Fagron	Hard fat	20G01-F02-376138	3
Fagron	Hard fat W35	20H17-B09-202675	3
Fagron	Hard fat W35	20J07-B02-202717	1
Fagron	Beeswax, white	2155	1
Fagron	Hard fat W35	21D14-B12	1
Fagron	Hard fat W35	21D14-B12-216502	1
Fagron	Hard fat W35	21D14-B12-219382	1
Fagron	Hard fat W35	21D14-B12-219988	1
Fagron	Hard fat W35	22D12-B01	2
Fagron	Hard fat W35	22D12-B01-220445	1
Fagron	Hard fat W35	22D12-B01-224504	1
Fagron	Hard fat	22H04-B02-222151	2
Fagron	Hard fat W35	22J26-B12-229479	1
Fagron	Beeswax, yellow	280A140306	1
Fagron	Hard fat	2OG01-F02-373358	1
Fagron	Hard fat W35	2OJ07-B02	1
Fagron	Hard fat W35	3518A-03934	1
Fagron	Hard fat W35	3914E-02328	1
Fagron	Hard fat W35	3917M-02328	1
Fagron	Hard fat	5628	1
Fagron	Hard fat	606469	1
Fagron	Hard fat W35	904381	1
Fagron	Hard fat	909394	2
Fagron	Hard fat W35	B02-2027107	1
Fagron	Hard fat W35	B0520134008	1
Fagron	Hard fat W35	B05-2013408	2
Fargon/Alliance HC	Cetyl palmitate	14351612	1
Fargon	Hard fat	2OG01-F02-372412	2
Fargon	Hard fat	41319264	1
Fiebig	Hard fat	20000906003	1
Finze	Beeswax, yellow	10145002	1
Fischer/Phönix	Cetyl palmitate	15301711	1
Gatt-Koller	Cocoa butter	1803838	1
Gehe	Hard fat	11345918	1
Gehe	Beeswax, yellow	12079412	1
Gehe	Beeswax, yellow	12367910	1
Gehe	Hard fat	13243403	1
GEHE	Beeswax, yellow	13335502	1
Gehe	Sodium dodecyl sulfate	14127404	1
Gehe	Paraffin, hard	14286511	1
Gehe	Beeswax, yellow	14336607	1
GEHE	Paraffin, hard	15295409	1
Gehe	Paraffin, hard	15295410	1
Gehe	Beeswax, yellow	16038207	1
GEHE	Beeswax, white	16163109	1
GEHE	Sodium dodecyl sulfate	16229205	1
GEHE	Hard fat	16274203	1
Gehe	Paraffin, microcrystalline	17137508	1
Gehe	Beeswax, yellow	18049001	1
GEHE	Beeswax, yellow	18113501	1
GEHE	Hard fat	18147901	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Cocoa butter	19036008	1
Gehe	Beeswax, white	191242004	1
Gehe	Beeswax, white	19124206	1
Gehe	Beeswax, yellow	19137202	1
Gehe	Hard fat	20003131008	1
Gehe	Paraffin, hard	21001748007	1
Gehe	Cetyl palmitate	22001785003	1
Gehe	Beeswax, yellow	22003888003	1
Gehe	Hard fat W35	22004876	1
Gehe	Sodium dodecyl sulfate	23000156007	2
gehe	Hard fat	23000561002	1
Gehe	Hard fat	23000561002	2
Gehe	Hard fat	23000561003	1
Gehe	Cetyl palmitate	8209646	1
Geibo	Beeswax, yellow	290A170915	1
Gutenberg-Apotheke	Cocoa butter	13292007	1
Hänseler	Beeswax, yellow		6
HCK	Paraffin, hard	16277705	1
Hedinger GmbH/Noweda	Paraffin, hard	17347701	1
Henry Lamotte/ Allia…	Cocoa butter	19036003	1
Hirsch	Beeswax, yellow	12257012	1
Ichthyol/Phönix	Sodium dodecyl sulfate	15344510	1
Ichthyol	Beeswax, yellow	13031239	1
Intern Drogen	Sodium dodecyl sulfate	216991080	1
INTERN-DROGEN	Hard fat	20003131003	1
INTERN-DROGEN	Beeswax, white	20003825001	2
INTERN-DROGEN	Beeswax, yellow	21001423005	1
INTERN-DROGEN	Paraffin, hard	21001748004	3
Jenne	Paraffin, hard	17347701	1
Jenne	Beeswax, white	22003630003	2
Jenne	Cetyl palmitate	23001428006	1
Jenne	Beeswax, white	23002638001	1
Kehr	Paraffin, hard	17347701	1
Kehr	Hard fat W35	17K09-B03-351980	1
Kehr	Beeswax, white	18048906	1
Kehr	Beeswax, yellow	18113501	1
Kehr	Beeswax, white	21001267012	1
Kehr	Beeswax, yellow	21004132003	2
Kehr	Beeswax, white	22003630003	2
Klenk	Beeswax, white	10503-01	1
Klenk	Beeswax, yellow	13335513	1
Klenk	Beeswax, yellow	160311	1
Klenk	Beeswax, white	19071005	1
Klenk	Beeswax, yellow	190A170314	1
Klenk	Beeswax, yellow	20110-01	1
Klenk	Beeswax, yellow	20110-03	1
Klenk	Beeswax, white	20609-01	2
Klenk	Beeswax, yellow	220110-002	1
Klenk	Beeswax, white	221115-001	1
Klenk	Beeswax, white	230413-001	1
Klenk	Beeswax, yellow	280A110110	1
Klenk	Beeswax, yellow	280A120627	5
Klenk	Beeswax, yellow	280-A120627	1
Klenk	Beeswax, yellow	280A130115	26
Klenk	Beeswax, yellow	280A13011A	1
Klenk	Beeswax, yellow	280A140306	7
Klenk	Beeswax, yellow	280A150528	13
Klenk	Beeswax, white	280A160311	17
Klenk	Beeswax, yellow	280A171019	31
Klenk	Beeswax, white	280A190715	18

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Beeswax, white	280A190715-01	1
Klenk	Beeswax, white	280A2008005-01	1
Klenk	Beeswax, white	280A200804	1
Klenk	Beeswax, white	280A200804-01	6
Klenk	Beeswax, white	280A200805-01	3
Klenk	Beeswax, white	280A210503-01	9
Klenk	Beeswax, white	280A220609-01	1
Klenk	Beeswax, white	280A220609-02	2
Klenk	Beeswax, white	280A221115-01	2
Klenk	Beeswax, yellow	282A120627	1
Klenk	Beeswax, yellow	282A140306	1
Klenk	Beeswax, yellow	290A081210	1
Klenk	Beeswax, yellow	290A110803	1
Klenk	Beeswax, yellow	290A120627	4
Klenk	Beeswax, yellow	290A140903	5
Klenk	Beeswax, yellow	290A150716	5
Klenk	Beeswax, yellow	290A151214	5
Klenk	Beeswax, yellow	290A170314	5
Klenk	Beeswax, yellow	290A170915	15
Klenk	Beeswax, yellow	290A200108-01	1
Klenk	Beeswax, yellow	290A200108-02	2
Klenk	Beeswax, yellow	290A220110-002	1
Klenk	Beeswax, yellow	290A220110-01	3
Klenk	Beeswax, yellow	290A220110-02	2
Klenk	Beeswax, yellow	290A230120-01	1
Klenk	Beeswax, yellow	290A230413-01	1
Klenk	Beeswax, yellow	416E01240	1
Klenk	Beeswax, white	804-01	1
Klenk	Beeswax, white	805-01	1
Krieger	Hard fat	23000447	1
L10	Cetyl palmitate	16053811	1
L10	Cetyl palmitate	16186805	1
L10	Beeswax, yellow	17207403	1
L12	Cocoa butter	16316508	1
L12	Paraffin, microcrystalline	17137502	1
L12	Beeswax, yellow	18113502	1
L12	Beeswax, yellow	18113506	1
L12	Cetyl palmitate	18149904	2
L30	Cetyl palmitate	17271505	1
L30	Paraffin, hard	17347701	1
Lamotte/Allia	Hard fat	18004024	1
Mittelwand bio 2017	Beeswax, yellow	5022017	1
Nachprüfung vom 31.0…	Hard fat	15185002	1
Nachprüfung	Cetyl palmitate	123456	1
Nachprüfung	Paraffin, hard	18070131	1
Nachprüfung	Cetyl palmitate	3012U01241	1
Nachprüfung	Cetyl palmitate	4917I-01242	1
Noweda	Cocoa butter	11117813	2
Noweda	Hard fat	11345909	1
Noweda	Paraffin, hard	11363206	1
Noweda	Beeswax, yellow	12124810	1
Noweda	Paraffin, microcrystalline	12266304	1
Noweda	Paraffin, hard	14286517	1
Noweda	Beeswax, yellow	150230004	1
Noweda	Beeswax, yellow	15023002	1
Noweda	Hard fat W35	16027801	1
Noweda	Beeswax, white	16163114	1
Noweda	Paraffin, hard	16277710	1
Noweda	Paraffin, hard	163277710	1
Noweda	Cetyl palmitate	17271505	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Paraffin, hard	17347701	1
Noweda	Hard fat W35	18006248	1
Noweda	Beeswax, white	18048901	1
noweda	Beeswax, yellow	18049001	1
Noweda	Hard fat	18147901	1
Noweda	Beeswax, white	18239106	1
Noweda	Hard fat	18333904	1
Noweda	Cetyl palmitate	19139004	1
Noweda	Beeswax, yellow	20000280008	2
Noweda	Beeswax, white	20000885007	1
Noweda	Beeswax, white	21001267002	3
Noweda	Beeswax, yellow	21001423001	2
Noweda	Beeswax, yellow	21001423003	1
Noweda	Beeswax, yellow	21001423005	1
Noweda	Paraffin, hard	21001748004	2
Noweda	Paraffin, hard	2100174801	1
Noweda	Paraffin, hard	21001748012	2
Noweda	Beeswax, white	22000795001	1
Noweda	Hard fat	23000561002	1
Noweda	Beeswax, yellow	280A120627	2
Noweda	Beeswax, yellow	290A23012001	1
Noweda	Beeswax, yellow	290A230120-01	1
Noweda	Beeswax, yellow	290A230413-01	1
Otto	Beeswax, yellow	WG10052021	1
Ph.Eur.	Beeswax, yellow	17207402	1
Pharmachem	Beeswax, white	15292014	1
Pharmachem	Beeswax, yellow	16038202	1
PHOENIX 24.07.2014	Beeswax, yellow	13001206	1
Phoenix 3.3.14	Hard fat	13243414	1
Phoenix goettingen 08.05	Beeswax, yellow	15098901	1
Phoenix goettingen 09.05	Paraffin, hard	13390415	1
Phoenix	Cetyl palmitate	14060705	1
Phoenix	Beeswax, white	15292003	1
Phoenix	Paraffin, hard	15295410	1
Phoenix	Beeswax, white	16163109	1
Phoenix	Hard fat W35	16k08-b10-332763	1
Phoenix	Cetyl palmitate	17164005	1
Phoenix	Paraffin, hard	18070131	1
Phoenix	Cetyl palmitate	18149912	1
Phoenix	Hard fat	18333904	1
Phoenix	Beeswax, white	19124206	1
Phoenix	Beeswax, yellow	20000280008	1
Phoenix	Paraffin, hard	21000732007	1
Phoenix	Beeswax, white	21001267002	1
Phoenix	Hard fat	21003046011	2
Phoenix	Cetyl palmitate	22001717001	1
Phoenix	Sodium dodecyl sulfate	23000156006	1
Phoenix	Beeswax, white	280A221115-01	1
Phoenix	Hard fat W35	3076	1
Phönix / 2	Beeswax, yellow	20000280002	1
Phönix, Caesar&Loret…	Beeswax, yellow	191372001	1
Phönix	Beeswax, yellow	10849001	1
Phönix	Beeswax, yellow	12367901	1
Phönix	Beeswax, yellow	12367904	1
Phönix	Beeswax, yellow	12367915	1
Phönix	Beeswax, yellow	13031206	1
Phönix	Cetyl palmitate	13131906	1
Phönix	Paraffin, microcrystalline	13274301	1
Phönix	Cetyl palmitate	13295919	1
phönix	Beeswax, white	15292022	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Phönix	Cetyl palmitate	15301711	1
Phönix	Beeswax, yellow	15317609	1
Phönix	Beeswax, yellow	16038206	2
phönix	Beeswax, yellow	16038207	1
phönix	Beeswax, white	16163109	1
Phönix	Hard fat	16274203	1
PHÖNIX	Beeswax, yellow	17011611	1
Phönix	Cetyl palmitate	17043504	1
Phönix	Cocoa butter	17314902	1
Phönix	Hard fat	18000346	1
Phönix	Beeswax, yellow	18049001	1
Phönix	Beeswax, yellow	18113501	1
Phönix	Cocoa butter	18135106	1
Phönix	Hard fat	18147902	2
Phönix	Cetyl palmitate	18149912	1
Phönix	Cocoa butter	19000676003	4
Phönix	Cocoa butter	19036011	3
Phönix	Cetyl palmitate	19139004	1
Phönix	Paraffin, hard	192463010	1
Phönix	Cetyl palmitate	192869002	1
Phönix	Cocoa butter	2000169002	1
Phönix	Beeswax, yellow	20003602005	1
Phönix	Beeswax, white	20003825001	1
Phönix	Paraffin, hard	21000732007	1
Phönix	Beeswax, yellow	21001423003	3
Phönix	Cetyl palmitate	22001717004	1
Phönix	Cocoa butter	27121	1
Phönix	Hard fat	277212	1
Phönix	Beeswax, white	280A171019	1
Phönix	Hard fat W35	B05-2013409	1
Phytocomm	Hard fat	209314	1
Purren Apotheke	Hard fat	10I03-N08	1
Rondell Apotheke	Hard fat	15185002	1
Sanacorp 03.01.22	Cetyl palmitate	220103CP	1
Sanacorp WE:18.04.16…	Beeswax, yellow	15023004	1
Sanacorp	Beeswax, yellow		1
Sanacorp	Cocoa butter	1121300203	1
Sanacorp	Beeswax, yellow	12257009	1
Sanacorp	Beeswax, yellow	12367910	1
Sanacorp	Cocoa butter	13027207	1
sanacorp	Cocoa butter	13140407	1
Sanacorp	Beeswax, yellow	13335502	1
Sanacorp	Beeswax, yellow	13378619	1
Sanacorp	Hard fat	14126203	1
sanacorp	Hard fat	14338703	1
Sanacorp	Beeswax, yellow	16038203	1
Sanacorp	Beeswax, white	16163105	1
Sanacorp	Beeswax, white	16163114	1
Sanacorp	Cetyl palmitate	16186805	1
Sanacorp	Hard fat	16274202	1
Sanacorp	Beeswax, yellow	17011604	2
Sanacorp	Beeswax, yellow	17011609	1
Sanacorp	Beeswax, yellow	17011612	1
Sanacorp	Cetyl palmitate	17043504	1
Sanacorp	Cocoa butter	17055908	3
Sanacorp	Cocoa butter	170559908	1
Sanacorp	Cetyl palmitate	17164004	1
Sanacorp	Cocoa butter	17314902	1
Sanacorp	Hard fat W35	17k09-b03-346709	1
Sanacorp	Paraffin, hard	18070131	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Beeswax, yellow	18113501	1
Sanacorp	Beeswax, yellow	18113502	1
Sanacorp	Cocoa butter	18135106	3
Sanacorp	Hard fat	18147907	1
Sanacorp	Beeswax, white	18239106	1
Sanacorp	Beeswax, yellow	18299201	1
Sanacorp	Beeswax, white	191242002	1
Sanacorp	Beeswax, yellow	191372001	1
Sanacorp	Beeswax, yellow	19137202	1
Sanacorp	Paraffin, hard	19246300	1
Sanacorp	Cetyl palmitate	192859003	1
Sanacorp	Cetyl palmitate	192859005	1
Sanacorp	Beeswax, yellow	20000280008	1
Sanacorp	Cetyl palmitate	20000975002	1
Sanacorp	Beeswax, white	20003825001	1
Sanacorp	Beeswax, yellow	21001423001	1
Sanacorp	Beeswax, yellow	21004132003	1
Sanacorp	Cetyl palmitate	22000395002	1
Sanacorp	Beeswax, white	22000795001	1
Sanacorp	Cetyl palmitate	22001717004	2
Sanacorp	Beeswax, yellow	22003888003	1
Sanacorp	Hard fat	23000561002	3
Sanacorp	Beeswax, white	280A171019	1
Sanacorp	Beeswax, yellow	290A230413-01	2
Sanacorp	Sodium dodecyl sulfate	5/AKD1	1
Sanacorp	Sodium dodecyl sulfate	5/AKD6	1
Sanacorp	Cetyl palmitate	8/AKD12	1
Sanacorp	Cetyl palmitate	8/AKD13	1
Sanacorp	Cocoa butter	AKD27	1
Sanacorp	Cocoa butter	AKD28	1
Spinnrad / Phönix	Cocoa butter	719300202	1
Spinnrad/ Noweda/ 08…	Cocoa butter	920300201	1
Spinnrad/ Sanacorp 2…	Cocoa butter	719300202	1
Spinnrad/GEHE	Cocoa butter	920300201	1
Spinnrad/Noweda	Beeswax, white	118048061	2
Spinnrad/Noweda	Cocoa butter	317300201	1
Spinnrad/Noweda	Cocoa butter	717300202	1
Spinnrad	Cocoa butter	1017300203	1
Spinnrad	Cocoa butter	1017300212	1
Spinnrad	Beeswax, white	1018048062	1
Spinnrad	Beeswax, white	1121402003	1
Spinnrad	Beeswax, white	118048061	1
spinnrad	Cocoa butter	1218300203	1
Spinnrad	Cocoa butter	221302051	1
Spinnrad	Beeswax, white	317048061	1
Spinnrad	Cocoa butter	319300201	1
spinnrad	Cocoa butter	3252	1
Spinnrad	Cocoa butter	512300202	1
spinnrad	Beeswax, white	718402002	1
Symbiotica	Cetyl palmitate	2208030-01	1
Unisan	Paraffin, hard	11166911	3
Wachs neu	Beeswax, yellow		2

- 230 341 spectra from 1515 *Apo-Ident* customers from a total of 48 157 batches from a further 713 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation results

The validation runs checked whether the substance/substance group *Waxes / Fats* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Waxes / Fats* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	2847	0	150 115
Type B	0	2198	5	199 881
Type C	0	5721	5	230 341

The substance/substance group *Waxes / Fats* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 99.7893 %)
Type B	100.0000 % (> 99.9912 %)	99.7730 % (> 99.6369 %)
Type C	100.0000 % (> 99.9007 %)	99.9127 % (> 99.8603 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
20865	20865	0.00	151.88
20986	20986	0.00	109.73
21067	22479	14.26	147.84
21433	23511	5.33	135.55
21482	24813	16.93	150.07
21483	21483	0.00	88.86
21682	21682	0.00	67.37
21731	22349	2.94	126.00
21766	22330	6.77	70.31
21875	23639	5.52	128.58
21880	21880	0.00	139.00
21984	21984	0.00	142.69
22244	23511	8.74	139.86
22245	23511	5.69	126.81
22325	21984	4.16	124.78
22330	22330	0.00	68.28

continued on the next page

continued from previous page

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22338	21880	5.97	138.52
22348	23067	7.52	142.80
22349	22349	0.00	129.49
22352	23278	13.73	102.80
22479	22479	0.00	142.34
22486	22486	0.00	113.40
22956	23511	19.71	137.96
23067	23067	0.00	146.24
23242	24715	12.53	102.45
23278	23278	0.00	98.05
23511	23511	0.00	131.08
23560	23817	7.32	127.85
23565	23067	44.60	146.04
23601	21880	5.59	139.15
23639	23639	0.00	122.66
23705	23067	45.23	147.01
23707	23067	6.57	146.32
23817	23817	0.00	111.94
24715	24715	0.00	95.22
24716	24716	0.00	96.68
24720	24720	0.00	138.15
24813	24813	0.00	148.94
24870	23511	4.42	135.82
25047	21880	13.55	140.32
25216	25216	0.00	93.48
25381	22479	23.83	146.37
25384	23067	6.02	153.74
25387	22349	7.54	144.35
25434	27418	14.29	138.17
25445	21880	9.03	140.46
25639	25639	0.00	142.58
25723	25723	0.00	76.72
25739	23511	18.08	106.37
26108	26108	0.00	94.37
26362	26362	0.00	140.62
26622	23511	38.42	159.61
26696	26696	0.00	95.62
26734	25723	19.04	101.51
26745	22349	6.38	128.80
26910	23511	8.25	114.97
26959	26959	0.00	112.86
27034	21880	17.15	141.39
27268	23511	19.72	106.98
27418	27418	0.00	144.55

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Wool alcohols**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20495-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Wool alcohols; Alcoholes lanae

Special notes

When selecting the *Wool alcohols* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Wool alcohols	6	2	21

Second-stage model

For differentiation of the substance/substance group *Wool alcohols* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Wool alcohols* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Glycerol monostearate, emulsifying	74.88	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Wool alcohols* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Wool alcohols*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Wool alcohols	13380601	21520	40	1412037
Caelo	Wool alcohols	153703	22328	60	20151111*
Caelo	Wool alcohols	153703	22329	60	20151111*
Caelo	Wool alcohols	163530	23098	40	20161223*
Caelo	Wool alcohols	191275	24722	40	20190606*
Caelo	Wool alcohols	22002307001	26302	40	20220805
Caelo	Wool alcohols	22002307001	26302SI	20	20220805
Caelo	Wool alcohols	24002633	27419	40	20241125*
Caelo	Wool alcohols	24002633	27419SI	20	20241125*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Type A All calibration spectra.

- 360 spectra of 9 reference samples from the substance/substance group *Wool alcohols*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 602 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 2 reference samples from the substance/substance group *Wool alcohols*.

- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Wool alcohols	173160	23972	40
Caelo	Wool alcohols	181619	24165	40

- 202 004 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 35 spectra from 22 *Apo-Ident* customers from 22 batches from the substance/substance group *Wool alcohols*.

- Among them are spectra of independent samples from 21 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Wool alcohols	11011401	1
Caelo	Wool alcohols	12340505	1
Caelo	Wool alcohols	13071502	1
Caelo	Wool alcohols	13083906	2
Caelo	Wool alcohols	13083912	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Wool alcohols	13226408	1
Caelo	Wool alcohols	13380601	1
Caelo	Wool alcohols	14262501	1
Caelo	Wool alcohols	15304502	1
Caelo	Wool alcohols	15304505	3
Caelo	Wool alcohols	17169701	3
Caelo	Wool alcohols	18092502	3
Caelo	Wool alcohols	18161904	1
Caelo	Wool alcohols	18161912	1
Caelo	Wool alcohols	19127504	2
Caelo	Wool alcohols	20002460003	1
Caelo	Wool alcohols	21002143004	1
Caelo	Wool alcohols	23101408	1
Caelo	Wool alcohols	4/2015	1
Caelo	Wool alcohols	6111801	1
Caesar & Loretz GmbH…	Wool alcohols	20002460003	1
Caesar & Loretz GmbH	Wool alcohols	18161904	1
Caesar & Loretz GmbH	Wool alcohols	19127504	1
Caesar & Loretz GmbH	Wool alcohols	20002460003	1
Cealo/ Noweda	Wool alcohols	13380601	1
Fagron	Wool alcohols	16235702	1
Noweda	Wool alcohols	22002784004	1

- 236 032 spectra from 1515 *Apo-Ident* customers from a total of 49 236 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Wool alcohols* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Wool alcohols* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	80	0	202 004
Type C	0	34	1	236 032

The substance/substance group *Wool alcohols* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9007 %)	97.1429 % (> 88.5714 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21520	21520	0.00	117.56
22328	22328	0.00	128.39
22329	22329	0.00	127.64
23098	23098	0.00	120.25
24722	24722	0.00	128.50
26302	24722	19.00	125.58
27419	27419	0.00	127.87

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Xylitol**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20994-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Xylitol; Xylitolum

Special notes

When selecting the *Xylitol* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Xylitol	7	5	24

Second-stage model

For differentiation of the substance/substance group *Xylitol* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Xylitol* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	70.16	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Xylitol* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Xylitol*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Xylitol	14068206	21755	60	20140317
Caelo	Xylitol	15135405	22248	60	20150417
Caelo	Xylitol	15135405	22579	40	20150417
Caelo	Xylitol	20002926	25619	40	20201027*
Caelo	Xylitol	23000539	26692	40	20230331*
Caelo	Xylitol	23000539	26692SI	20	20230331*
Caelo	Xylitol	24000699	27256	40	20240411*
Caelo	Xylitol	24000699	27256SI	20	20240411*
Fagron	Xylitol	14G04-B04-298356	21754	60	AR-15-FG-008046-01
Fagron	Xylitol	14G04-B04-303524	22254	60	20140919

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 440 spectra of 10 reference samples from the substance/substance group *Xylitol*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

batches.

- 152 522 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 210 spectra of 6 reference samples from the substance/substance group *Xylitol*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Xylitol	15388101	22578	40
Caelo	Xylitol	163174	23061	40
Caelo	Xylitol	181133	24041	40
Caelo	Xylitol	21004147	26002	40
Caelo	Xylitol	24002073	27306	40
Caelo	Xylitol	21004147	26002SI	10

- 201 874 spectra from a total of 4040 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 40 spectra from 19 *Apo-Ident* customers from 27 batches from the substance/substance group *Xylitol*.

- Among them are spectra of independent samples from 24 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Xylitol	23000699002	1
Caelo	Xylitol	1219Q-02787	1
Caelo	Xylitol	12240612	1
Caelo	Xylitol	13230302	1
Caelo	Xylitol	13230305	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Xylitol	13230309	1
Caelo	Xylitol	13230315	1
Caelo	Xylitol	14061401	1
Caelo	Xylitol	14068206	1
Caelo	Xylitol	14G04-B04-298356	2
Caelo	Xylitol	15388104	3
Caelo	Xylitol	16317401	1
Caelo	Xylitol	18045302	4
Caelo	Xylitol	18113304	1
Caelo	Xylitol	18235908	1
Caelo	Xylitol	19120404	2
Caelo	Xylitol	20003607001	2
Caelo	Xylitol	3314M-02787	1
Caelo	Xylitol	5112I-02787	1
Caelo	Xylitol	718I-02787	1
Caesar & Loretz GmbH	Xylitol	20003607001	2
Caesar & Loretz GmbH	Xylitol	20003607013	1
Fagron	Xylitol	12J25-N06	2
Fagron	Xylitol	13/23-N06	1
Fagron	Xylitol	13H28N10	1
Fagron	Xylitol	13H28-N10	2
Fagron	Xylitol	14G04-B04-303524	2
Fagron	Xylitol	16c14-B02-320887	1

- 236 027 spectra from 1515 *Apo-Ident* customers from a total of 49 231 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Xylitol* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xylitol* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	440	0	152 522
Type B	0	210	0	201 874
Type C	0	40	0	236 027

The substance/substance group *Xylitol* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.6364 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 97.1429 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 85.0000 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21754	21754	0.00	187.37
21755	26692	6.79	182.74
22248	26692	6.20	182.56
22254	21754	5.48	184.62
22579	27256	6.90	185.07
25619	25619	0.00	183.26
26692	26692	0.00	182.03
27256	27256	0.00	185.29

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Xylometazoline hydrochloride**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20025-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Xylometazoline hydrochloride; Xylometazolini hydrochloridum

Special notes

When selecting the *Xylometazoline hydrochloride* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.

2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.

3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Xylometazoline hydrochloride	7	5	82

Second-stage model

For differentiation of the substance/substance group *Xylometazoline hydrochloride* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Xylometazoline hydrochloride* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Ornithine aspartate	64.74	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Xylometazoline hydrochloride* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Xylometazoline hydrochloride*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Xylometazoline hydrochloride	13344901	21516	60	1501655
Caelo	Xylometazoline hydrochloride	13344901	21517	60	20131119
Caelo	Xylometazoline hydrochloride	16074211	23246	40	20160318
Fagron	Xylometazoline hydrochloride	13I18-B03-295481	21722	60	AR-15-FG-007785-01
Fagron	Xylometazoline hydrochloride	14K19-B05-305006	21927	60	20141128
Fagron	Xylometazoline hydrochloride	14K19-B05-305006	21927SI	60	20141128
Fagron	Xylometazoline hydrochloride	19B07-B02-373357	25735	40	20190408
Fagron	Xylometazoline hydrochloride	19B07-B02-373357	25735SI	40	20190408
Fagron	Xylometazoline hydrochloride	21K10-B04-215749	26060	40	20211207
Fagron	Xylometazoline hydrochloride	21K10-B04-215749	26060SI	40	20211207
Fagron	Xylometazoline hydrochloride	23L07-B05-227259	27047	40	20231213

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 540 spectra of 11 reference samples from the substance/substance group *Xylometazoline - hydrochloride*. These samples are listed above in the *calibration samples* section. The reference samples come from 7 different batches.

- 152 422 spectra from a total of 2835 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 620 spectra of 15 reference samples from the substance/substance group *Xylometazoline hydrochloride*.

- Among them are spectra of independent samples from 5 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Xylometazoline hydrochloride	170739	23314	40
Caelo	Xylometazoline hydrochloride	173457	23832	40
Caelo	Xylometazoline hydrochloride	21000078002	25734	40
Caelo	Xylometazoline hydrochloride	22000302	26023	40
Caelo	Xylometazoline hydrochloride	24001236	27315	40
Caelo	Xylometazoline hydrochloride	13344901	21517SI†	60
Caelo	Xylometazoline hydrochloride	16074211	23246SI†	40
Caelo	Xylometazoline hydrochloride	170739	23314SI	40
Caelo	Xylometazoline hydrochloride	170739	23320	40
Caelo	Xylometazoline hydrochloride	170739	23320SI	40
Caelo	Xylometazoline hydrochloride	173457	23832SI	40
Caelo	Xylometazoline hydrochloride	21000078002	25734SI	40
Caelo	Xylometazoline hydrochloride	22000302	26023SI	40
Caelo	Xylometazoline hydrochloride	24001236	27315SI	40
Fagron	Xylometazoline hydrochloride	23L07-B05-227259	27047SI†	40

- 201 464 spectra from a total of 4037 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

provided by the customer regarding manufacturer and batch number.

- 258 spectra from 172 *Apo-Ident* customers from 84 batches from the substance/substance group *Xylometazoline hydrochloride*.
- Among them are spectra of independent samples from 82 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Xylometazoline hydrochloride	22000302001	2
	Xylometazoline hydrochloride	22000302006	1
	Xylometazoline hydrochloride	22000302010	1
	Xylometazoline hydrochloride	2200302004	1
	Xylometazoline hydrochloride	23002949001	1
	Xylometazoline hydrochloride	23002949004	1
Alliance	Xylometazoline hydrochloride	192761007	2
Alliance	Xylometazoline hydrochloride	22000302004	1
Anzag	Xylometazoline hydrochloride	12027911	1
Anzag	Xylometazoline hydrochloride	15037907	2
Caelo	Xylometazoline hydrochloride	10118821	2
Caelo	Xylometazoline hydrochloride	12027906	2
Caelo	Xylometazoline hydrochloride	12287201	2
Caelo	Xylometazoline hydrochloride	12287203	8
Caelo	Xylometazoline hydrochloride	12287204	2
Caelo	Xylometazoline hydrochloride	12287210	7
Caelo	Xylometazoline hydrochloride	12287212	2
Caelo	Xylometazoline hydrochloride	12287213	1
Caelo	Xylometazoline hydrochloride	13171202	10
Caelo	Xylometazoline hydrochloride	13171203	2
Caelo	Xylometazoline hydrochloride	13171205	1
Caelo	Xylometazoline hydrochloride	13344901	1
Caelo	Xylometazoline hydrochloride	13344908	1
Caelo	Xylometazoline hydrochloride	15037906	1
Caelo	Xylometazoline hydrochloride	15037907	4
Caelo	Xylometazoline hydrochloride	15037910	2
Caelo	Xylometazoline hydrochloride	15037912	1
Caelo	Xylometazoline hydrochloride	15292803	3
Caelo	Xylometazoline hydrochloride	15292804	5
Caelo	Xylometazoline hydrochloride	15292811	1
Caelo	Xylometazoline hydrochloride	15292812	2
Caelo	Xylometazoline hydrochloride	153037907	1
Caelo	Xylometazoline hydrochloride	160740209	1
Caelo	Xylometazoline hydrochloride	16074201	4
Caelo	Xylometazoline hydrochloride	16074202	2
Caelo	Xylometazoline hydrochloride	16074205	6
Caelo	Xylometazoline hydrochloride	16074209	8
Caelo	Xylometazoline hydrochloride	160742095416	1
Caelo	Xylometazoline hydrochloride	16074216	3
Caelo	Xylometazoline hydrochloride	16074217	3
Caelo	Xylometazoline hydrochloride	16322082	1
Caelo	Xylometazoline hydrochloride	1703902	1
Caelo	Xylometazoline hydrochloride	1703909	1
Caelo	Xylometazoline hydrochloride	17073902	3
Caelo	Xylometazoline hydrochloride	17073905	8
Caelo	Xylometazoline hydrochloride	17073908	1
Caelo	Xylometazoline hydrochloride	17073909	4
Caelo	Xylometazoline hydrochloride	17344512	1
Caelo	Xylometazoline hydrochloride	17345703	12
Caelo	Xylometazoline hydrochloride	17345706	2
Caelo	Xylometazoline hydrochloride	17345707	3
Caelo	Xylometazoline hydrochloride	17345708	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Xylometazoline hydrochloride	17345712	4
Caelo	Xylometazoline hydrochloride	181102181	1
Caelo	Xylometazoline hydrochloride	192751007	1
Caelo	Xylometazoline hydrochloride	192761005	15
Caelo	Xylometazoline hydrochloride	192761007	7
Caelo	Xylometazoline hydrochloride	2031502	1
Caelo	Xylometazoline hydrochloride	21000078001	1
Caelo	Xylometazoline hydrochloride	21000078002	2
Caelo	Xylometazoline hydrochloride	21000078003	2
Caelo	Xylometazoline hydrochloride	21000078004	3
Caelo	Xylometazoline hydrochloride	2100078001	1
Caelo	Xylometazoline hydrochloride	2100078004	1
Caelo	Xylometazoline hydrochloride	21003217001	2
Caelo	Xylometazoline hydrochloride	21003217002	4
Caelo	Xylometazoline hydrochloride	2200030004	1
Caelo	Xylometazoline hydrochloride	22000302004	3
Caelo	Xylometazoline hydrochloride	22000302008	1
Caelo	Xylometazoline hydrochloride	220003302003	1
Caelo	Xylometazoline hydrochloride	23051820	1
Caelo	Xylometazoline hydrochloride	24111202	1
Caelo	Xylometazoline hydrochloride	9276404	1
Caelo	Xylometazoline hydrochloride	9278404	1
Caesar & Loretz GmbH...	Xylometazoline hydrochloride	21000078002	1
Caesar & Loretz GmbH...	Xylometazoline hydrochloride	21000078004	1
Caesar & Loretz GmbH...	Xylometazoline hydrochloride	17345712	1
Caesar & Loretz GmbH...	Xylometazoline hydrochloride	192761005	1
Caesar & Loretz GmbH...	Xylometazoline hydrochloride	17345710	1
Caesar & Loretz GmbH...	Xylometazoline hydrochloride	192761005	1
Caesar & Loretz GmbH	Xylometazoline hydrochloride	17073902	1
Caesar & Loretz GmbH	Xylometazoline hydrochloride	17345706	1
Caesar & Loretz GmbH	Xylometazoline hydrochloride	17345707	1
Caesar & Loretz GmbH	Xylometazoline hydrochloride	17345708	3
Caesar & Loretz GmbH	Xylometazoline hydrochloride	17345710	3
Caesar & Loretz GmbH	Xylometazoline hydrochloride	17345712	1
Caesar & Loretz GmbH	Xylometazoline hydrochloride	192761007	2
Caesar & Loretz GmbH	Xylometazoline hydrochloride	21000078001	2
Caesar & Loretz GmbH	Xylometazoline hydrochloride	21000078004	7
Caesar & Loretz GmbH	Xylometazoline hydrochloride	21003217002	4
Caesar & Loretz GmbH	Xylometazoline hydrochloride	22000302001	1
Celoa vdL	Xylometazoline hydrochloride	13171202	1
Fagron	Xylometazoline hydrochloride	10416XMHC	1
Fagron	Xylometazoline hydrochloride	12287210	1
Fagron	Xylometazoline hydrochloride	12G31-N01	1
Fagron	Xylometazoline hydrochloride	13171203	1
Fagron	Xylometazoline hydrochloride	1318-B03-295479	1
Fagron	Xylometazoline hydrochloride	13E06-N11	1
Fagron	Xylometazoline hydrochloride	13I09-N02	1
Fagron	Xylometazoline hydrochloride	15Jo6-B99-313751	1
Fagron	Xylometazoline hydrochloride	15K25-B07-318956	1
Fagron	Xylometazoline hydrochloride	21K10-B04-215749	1
Gehe	Xylometazoline hydrochloride	10118802	1
Gehe	Xylometazoline hydrochloride	16074201	1
GEHE	Xylometazoline hydrochloride	16074209	1
Gehe	Xylometazoline hydrochloride	17345703	1
Geilenkirchen	Xylometazoline hydrochloride	16074209	1
Geilenkirchen	Xylometazoline hydrochloride	17345708	1
InfectoPharm/Gehe	Xylometazoline hydrochloride	17345707	1
Nachprüfung	Xylometazoline hydrochloride	4317E-03337	1
Noweda	Xylometazoline hydrochloride	12027902	1
Noweda	Xylometazoline hydrochloride	12287203	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Xylometazoline hydrochloride	17345708	1
Phönix	Xylometazoline hydrochloride	22000302003	1
Sanacorp	Xylometazoline hydrochloride	12027902	1
Sanacorp	Xylometazoline hydrochloride	15037906	1
Sanacorp	Xylometazoline hydrochloride	17345703	1
sanacorp	Xylometazoline hydrochloride	22000302003	1
Siegrfried Pharma Ch…	Xylometazoline hydrochloride	22000302008	1

- 235 809 spectra from 1515 *Apo-Ident* customers from a total of 49 174 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Xylometazoline hydrochloride* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xylometazoline hydrochloride* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	540	0	152 422
Type B	0	620	0	201 464
Type C	0	257	1	235 809

The substance/substance group *Xylometazoline hydrochloride* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.8889 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.0323 %)
Type C	100.0000 % (> 99.9007 %)	99.6124 % (> 98.4496 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21516	21516	0.00	82.99
21517	21516	5.39	84.11
21722	21722	0.00	86.68
21927	21722	7.81	87.86
23246	21722	6.42	85.05
25735	21722	10.97	86.48
26060	21722	8.77	86.21
27047	21722	19.61	87.93

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Xylose**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20517-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Xylose; Xylosum

Special notes

When selecting the *Xylose* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Xylose	6	7	27

Second-stage model

For differentiation of the substance/substance group *Xylose* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Xylose* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	81.21	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Xylose* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Xylose*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Xylose	14218902	21606	60	AR-14-FG-013086-01
Caelo	Xylose	17160902	23413	40	20170704
Caelo	Xylose	191802002	25437	40	20190819
Caelo	Xylose	21000133001	25732	50	20210219
Fagron	Xylose	13A31-B40-292395	21763	60	20140407
Fagron	Xylose	16A25-B05-328261	23524	40	20160215

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 290 spectra of 6 reference samples from the substance/substance group *Xylose*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 672 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 310 spectra of 9 reference samples from the substance/substance group *Xylose*.
- Among them are spectra of independent samples from 7 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Xylose	13133402	20868	40
Caelo	Xylose	162064	22758	40
Caelo	Xylose	171609	23656	40
Caelo	Xylose	173188	23849	40
Caelo	Xylose	190499	24527	40
Caelo	Xylose	22000045004	26310	30
Caelo	Xylose	23000619	27123	40
Caelo	Xylose	22000045004	26310SI	20
Caelo	Xylose	23000619	27123SI	20

- 201 774 spectra from a total of 4038 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 45 spectra from 15 *Apo-Ident* customers from 29 batches from the substance/substance group *Xylose*.
- Among them are spectra of independent samples from 27 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Xylose	23000619001	2
Caelo	Xylose	11031501	1
Caelo	Xylose	12120101	1
Caelo	Xylose	13133404	2
Caelo	Xylose	13133410	1
Caelo	Xylose	13133414	3
Caelo	Xylose	16002301	1
Caelo	Xylose	16002302	2
Caelo	Xylose	16002309	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Xylose	16206405	1
Caelo	Xylose	17160902	2
Caelo	Xylose	17160905	2
Caelo	Xylose	17318803	4
Caelo	Xylose	17318809	1
Caelo	Xylose	19049902	1
Caelo	Xylose	19180205	2
Caelo	Xylose	21000133002	1
Caelo	Xylose	5031501	1
Caesar & Loretz GmbH	Xylose	20000783003	2
Ebert & Jacobi 12…	Xylose	16002301	2
Eigenherstellung	Xylose	80414HJK01	1
Euro OTC	Xylose		1
Fagron	Xylose	10121401	1
Fagron	Xylose	13133415	1
Fagron	Xylose	14E-B03_300658	1
Fagron	Xylose	28111405	1
Fagron	Xylose	80414PJK01	1
Falcento	Xylose	2013051801	1
Phoenix 20.06.2014	Xylose	13A31-B04-292396	1
Phoenix Goettin	Xylose	13133422	1

- 236 022 spectra from 1515 *Apo-Ident* customers from a total of 49 229 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Xylose* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Xylose* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	290	0	152 672
Type B	0	310	0	201 774
Type C	0	45	0	236 022

The substance/substance group *Xylose* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.9310 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 98.0645 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 86.6667 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21606	21606	0.00	155.42
21763	21606	21.01	156.70
23413	21606	17.27	157.75
23524	21606	18.77	154.33
25437	21606	27.27	176.50
25732	21606	18.50	168.18

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Zinc acetate dihydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20398-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Zinc acetate dihydrate; Zinci acetas dihydricus

Special notes

When selecting the *Zinc acetate dihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Zinc acetate dihydrate	6	3	29

Second-stage model

For differentiation of the substance/substance group *Zinc acetate dihydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Zinc acetate dihydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Carbomers	93.74	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Zinc acetate dihydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Zinc acetate dihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Zinc acetate dihydrate	15383301	22728	40	20151127
Caelo	Zinc acetate dihydrate	153833	23030	40	20151127*
Caelo	Zinc acetate dihydrate	170204	23031	40	20170126*
Caelo	Zinc acetate dihydrate	170204	23637	40	20172601*
Caelo	Zinc acetate dihydrate	19000422	25208	40	20191230*
Caelo	Zinc acetate dihydrate	21000302	25652	40	20210303*
Caelo	Zinc acetate dihydrate	22002583	26479	30	20221109*
Caelo	Zinc acetate dihydrate	22002583	26479SI	20	20221109*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 290 spectra of 8 reference samples from the substance/substance group *Zinc acetate dihydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 6 different batches.

- 152 672 spectra from a total of 2836 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 140 spectra of 4 reference samples from the substance/substance group *Zinc acetate dihydrate*.

- Among them are spectra of independent samples from 3 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Zinc acetate dihydrate	17020404	23514	40
Caelo	Zinc acetate dihydrate	182046	24213	40
Caelo	Zinc acetate dihydrate	23001173	26895	40
Caelo	Zinc acetate dihydrate	23001173	26895SI	20

- 201 944 spectra from a total of 4042 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 99 spectra from 82 *Apo-Ident* customers from 30 batches from the substance/substance group *Zinc acetate dihydrate*.

- Among them are spectra of independent samples from 29 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Zinc acetate dihydrate	21000302011	1
	Zinc acetate dihydrate	22002583004	1
	Zinc acetate dihydrate	22002583006	1
	Zinc acetate dihydrate	22002583010	1
Caelo	Zinc acetate dihydrate	12134801	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Zinc acetate dihydrate	12134803	1
Caelo	Zinc acetate dihydrate	12316401	2
Caelo	Zinc acetate dihydrate	12316403	2
Caelo	Zinc acetate dihydrate	12316404	2
Caelo	Zinc acetate dihydrate	12316405	1
Caelo	Zinc acetate dihydrate	14133201	1
Caelo	Zinc acetate dihydrate	15160801	1
Caelo	Zinc acetate dihydrate	15160804	1
Caelo	Zinc acetate dihydrate	15383304	1
Caelo	Zinc acetate dihydrate	15383306	4
Caelo	Zinc acetate dihydrate	15383308	2
Caelo	Zinc acetate dihydrate	17020403	3
Caelo	Zinc acetate dihydrate	17020404	3
Caelo	Zinc acetate dihydrate	17197601	9
Caelo	Zinc acetate dihydrate	17365807	1
Caelo	Zinc acetate dihydrate	18204604	6
Caelo	Zinc acetate dihydrate	18204610	1
Caelo	Zinc acetate dihydrate	19000422007	4
Caelo	Zinc acetate dihydrate	19000422011	1
Caelo	Zinc acetate dihydrate	20004443001	2
Caelo	Zinc acetate dihydrate	21000302002	2
Caelo	Zinc acetate dihydrate	21000302006	5
Caelo	Zinc acetate dihydrate	21000302011	1
Caelo	Zinc acetate dihydrate	22002583004	5
Caesar & Loretz GmbH...	Zinc acetate dihydrate	19000422011	1
Caesar & Loretz GmbH...	Zinc acetate dihydrate	18204610	1
Caesar & Loretz GmbH...	Zinc acetate dihydrate	22002583004	1
Caesar & Loretz GmbH/Kehr	Zinc acetate dihydrate	20004443001	1
Caesar & Loretz GmbH	Zinc acetate dihydrate	18204604	2
Caesar & Loretz GmbH	Zinc acetate dihydrate	19000422007	1
Caesar & Loretz GmbH	Zinc acetate dihydrate	19000422011	4
Caesar & Loretz GmbH	Zinc acetate dihydrate	21000302002	2
Caesar & Loretz GmbH	Zinc acetate dihydrate	21000302006	4
Caesar & Loretz GmbH	Zinc acetate dihydrate	21000302014	1
Caesar & Loretz GmbH	Zinc acetate dihydrate	22002583004	2
Caesar & Loretz GmbH	Zinc acetate dihydrate	22002583006	1
Caesar/Sanacorp	Zinc acetate dihydrate	18204604	1
Cealo	Zinc acetate dihydrate	17197601	1
Euro OTC	Zinc acetate dihydrate	15383301	1
Gehe	Zinc acetate dihydrate	17020404	1
Noweda	Zinc acetate dihydrate	18204604	1
phönix	Zinc acetate dihydrate	15383301	1
Phönix	Zinc acetate dihydrate	17197601	1
PHÖNIX	Zinc acetate dihydrate	19000422011	1
Phönix	Zinc acetate dihydrate	2200253006	1
phönix	Zinc acetate dihydrate	22002583004	1
Sanacorp	Zinc acetate dihydrate	19000422011	1

- 235 968 spectra from 1515 *Apo-Ident* customers from a total of 49 229 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Zinc acetate dihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose,

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

all relevant spectra of the various substances were compared with *Zinc acetate dihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	290	0	152 672
Type B	0	140	0	201 944
Type C	0	98	1	235 968

The substance/substance group *Zinc acetate dihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 97.9310 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 95.7143 %)
Type C	100.0000 % (> 99.9007 %)	98.9899 % (> 95.9596 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
22728	23030	4.38	157.17
23030	23030	0.00	157.04
23031	23031	0.00	154.41
23637	23637	0.00	154.51
25208	25208	0.00	156.65
25652	25652	0.00	152.21
26479	26479	0.00	152.69

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Zinc gluconate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20379-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Zinc gluconate; Zinci gluconas

Special notes

When selecting the *Zinc gluconate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Zinc gluconate	8	17	56

Second-stage model

For differentiation of the substance/substance group *Zinc gluconate* the following second-stage model is used:

- Submodel 04

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Zinc gluconate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Polymyxin B sulfate	55.50	–
⋮	⋮	⋮
Tobramycin sulfate	>50	28.46
Neomycin sulfate	>50	55.29
Riboflavin sodium phosphate hydrate	>50	55.50
Gentamicin sulfate	>50	74.50
Magnesium citrate	>50	85.11
Carbomers	>50	117.96
Mg-Ca-K colamine phosphate	>50	122.17
Sodium tetraborate	>50	302.29
Finasteride	>50	1654.12

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Zinc gluconate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Zinc gluconate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Zinc gluconate	170165	23034	40	20170125*
Caelo	Zinc gluconate	170951	23292	40	20170518*
Euro OTC	Zinc gluconate	1407033-02	21709	60	20140902
Euro OTC	Zinc gluconate	1508007	21882	60	20150827*
Euro OTC	Zinc gluconate	1603035	22513	40	20160427*
Euro OTC	Zinc gluconate	1807019	24150	40	20180725*
Euro OTC	Zinc gluconate	2007007	25318	40	20200826*
Euro OTC	Zinc gluconate	2103006	25603	40	20210323*

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 360 spectra of 8 reference samples from the substance/substance group *Zinc gluconate*. These samples are listed above in the *calibration samples* section. The reference samples come from 8 different batches.

- 152 602 spectra from a total of 2834 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 760 spectra of 21 reference samples from the substance/substance group *Zinc gluconate*.

- Among them are spectra of independent samples from 17 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Zinc gluconate	161788	22619	40
Caelo	Zinc gluconate	20002679	25611	40
Caelo	Zinc gluconate	23001539	26893	40
Euro OTC	Zinc gluconate	1606018	22700	40
Euro OTC	Zinc gluconate	1701017	22994	40
Euro OTC	Zinc gluconate	1706009	23544	40
Euro OTC	Zinc gluconate	1711004	23730	40
Euro OTC	Zinc gluconate	1810014	24347	40
Euro OTC	Zinc gluconate	1902017	24635	40
Euro OTC	Zinc gluconate	1910010	24942	40
Euro OTC	Zinc gluconate	2007027	25316	40
Euro OTC	Zinc gluconate	2110001	25887	50
Euro OTC	Zinc gluconate	2208029	26338	40
Euro OTC	Zinc gluconate	2302019	26641	40
Euro OTC	Zinc gluconate	2312003	27074	40
Euro OTC	Zinc gluconate	2405017	27293	40
Fagron	Zinc gluconate	22L30-B04-225958	26919	40
Caelo	Zinc gluconate	23001539	26893SI	20
Euro OTC	Zinc gluconate	2110001	25887SI	10
Euro OTC	Zinc gluconate	2208029	26338SI	20
Euro OTC	Zinc gluconate	2302019	26641SI	20

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

- 201 324 spectra from a total of 4028 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 447 spectra from 22 *Apo-Ident* customers from 58 batches from the substance/substance group *Zinc gluconate*.

- Among them are spectra of independent samples from 56 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
	Zinc gluconate	2312003-01	1
	Zinc gluconate	23C22-B09	2
	Zinc gluconate	7500200698	1
Caelo	Zinc gluconate	16001601	1
Caelo	Zinc gluconate	16178801	1
Caelo	Zinc gluconate	17016502	3
Caelo	Zinc gluconate	17095103	1
Caelo	Zinc gluconate	18069506	1
Caelo	Zinc gluconate	18069511	1
Caelo	Zinc gluconate	19044602	3
Caelo	Zinc gluconate	19044603	2
Caelo	Zinc gluconate	19044607	1
Caelo	Zinc gluconate	191451002	1
Caelo	Zinc gluconate	19145103	1
Caelo	Zinc gluconate	20000647001	1
Caelo	Zinc gluconate	20000647002	1
Caelo	Zinc gluconate	20002679003	1
Caelo	Zinc gluconate	20002679004	1
Caelo	Zinc gluconate	20003987	1
Caelo	Zinc gluconate	20003987001	3
Caelo	Zinc gluconate	20003987002	1
Caelo	Zinc gluconate	20003987005	1
Caelo	Zinc gluconate	21003511001	3
Caelo	Zinc gluconate	21003511003	2
Caelo	Zinc gluconate	22003957003	3
Caelo	Zinc gluconate	23001539001	1
Caelo	Zinc gluconate	23003413002	1
Caesar & Loretz GmbH	Zinc gluconate	19044607	1
Caesar & Loretz GmbH	Zinc gluconate	20003987004	1
Euro OTC	Zinc gluconate	1312010-01	1
Euro OTC	Zinc gluconate	1405011-01	1
Euro OTC	Zinc gluconate	1508007-01	16
Euro OTC	Zinc gluconate	1508007-02	40
Euro OTC	Zinc gluconate	1603035-01	40
Euro OTC	Zinc gluconate	1606018-01	34
Euro OTC	Zinc gluconate	1606018-02	36
Euro OTC	Zinc gluconate	1701017-01	31
Euro OTC	Zinc gluconate	1706009-01	66
Euro OTC	Zinc gluconate	170901201	9
Euro OTC	Zinc gluconate	1709012-0103707875	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Zinc gluconate	1711004-01	28
Euro OTC	Zinc gluconate	1807019	1
Euro OTC	Zinc gluconate	1807019-01	14
Euro OTC	Zinc gluconate	1810014-01	1
Euro OTC	Zinc gluconate	1902017-01	1
Euro OTC	Zinc gluconate	1902018-01	5
Euro OTC	Zinc gluconate	191001001	1
Euro OTC	Zinc gluconate	1910010-01	2
Euro OTC	Zinc gluconate	2007007	1
Euro OTC	Zinc gluconate	2007007-01	6
Euro OTC	Zinc gluconate	2007027-01	19
Euro OTC	Zinc gluconate	2103006-01	9
Euro OTC	Zinc gluconate	211000101	1
Euro OTC	Zinc gluconate	2110001-01	8
Euro OTC	Zinc gluconate	27061711	1
Euro OTC	Zinc gluconate	ZGE-USP2004028	1
Fagron	Zinc gluconate	14J30-B06-300520	1
Fagron	Zinc gluconate	20G06-F01-372826	1
Fagron	Zinc gluconate	22A21-B08-216993	1
KOKO Gmbh	Zinc gluconate	1810014-01	28

- 235 620 spectra from 1515 *Apo-Ident* customers from a total of 49 201 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Zinc gluconate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zinc gluconate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	360	0	152 602
Type B	0	760	0	201 324
Type C	0	447	0	235 620

The substance/substance group *Zinc gluconate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 98.3333 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 99.2105 %)
Type C	100.0000 % (> 99.9007 %)	100.0000 % (> 98.6577 %)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21709	25603	5.52	63.42
21882	21882	0.00	63.84
22513	22513	0.00	72.05
23034	23034	0.00	61.33
23292	23292	0.00	61.85
24150	24150	0.00	69.83
25318	25318	0.00	61.76
25603	25603	0.00	66.11

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Zinc orotate dihydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	20424-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Zinc orotate dihydrate; Zincum oroticum dihydricum

Special notes

When selecting the *Zinc orotate dihydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Zinc orotate dihydrate	3	1	1

Second-stage model

For differentiation of the substance/substance group *Zinc orotate dihydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Zinc orotate dihydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Aluminium chloride hexahydrate	86.40	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Zinc orotate dihydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Zinc orotate dihydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Zinc orotate dihydrate	1203014-01	21038	40	1407431
Euro OTC	Zinc orotate dihydrate	13050005-02	21326	40	20130628*
Euro OTC	Zinc orotate dihydrate	2312002	26993	40	20231214*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 120 spectra of 3 reference samples from the substance/substance group *Zinc orotate dihydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 3 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 842 spectra from a total of 2839 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 80 spectra of 3 reference samples from the substance/substance group *Zinc orotate dihydrate*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Euro OTC	Zinc orotate dihydrate	2302021	26631	40
Euro OTC	Zinc orotate dihydrate	2302021	26631SI	20
Euro OTC	Zinc orotate dihydrate	2312002	26993SI†	20

- 202 004 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Zinc orotate dihydrate*.
- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Ichtyol/Phönix	Zinc orotate dihydrate	12B02-N02	1

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are docu-

†These spectra were recorded from material of the same package as the corresponding calibration spectra (*Type A*). Hence, these spectra are not independent and are not of *Type B*.

mented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Zinc orotate dihydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zinc orotate dihydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	120	0	152 842
Type B	0	80	0	202 004
Type C	0	0	1	236 066

The substance/substance group *Zinc orotate dihydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 92.5000 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
21038	21038	0.00	231.09
21326	21326	0.00	238.47
26993	26993	0.00	152.27

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Zinc stearate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	24018-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Zinc stearate; Zinci stearas

Special notes

When selecting the *Zinc stearate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Zinc stearate	2	1	1

Second-stage model

For differentiation of the substance/substance group *Zinc stearate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Zinc stearate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Cetyl palmitate	33.14	–
Beeswax, white	35.94	–
Paraffin, hard	37.98	–
Beeswax, yellow	38.21	–
Hard fat	50.80	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Zinc stearate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Zinc stearate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Caelo	Zinc stearate	180628	24018	40	20180322*
Caelo	Zinc stearate	22000651	26123	40	20220426*
Caelo	Zinc stearate	22000651	26123SI	20	20220426*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 100 spectra of 3 reference samples from the substance/substance group *Zinc stearate*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

- 152 862 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 40 spectra of 1 reference samples from the substance/substance group *Zinc stearate*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Zinc stearate	182279	24500	40

- 202 044 spectra from a total of 4044 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 1 spectra from 1 *Apo-Ident* customers from 1 batches from the substance/substance group *Zinc stearate*.

- Among them are spectra of independent samples from 1 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Zinc stearate	22002130001	1

- 236 066 spectra from 1515 *Apo-Ident* customers from a total of 49 257 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model,

the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Zinc stearate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zinc stearate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type ($A/B/C$).

	False positive	True positive	False negative	True negative
Type A	0	100	0	152 862
Type B	0	40	0	202 044
Type C	0	1	0	236 066

The substance/substance group *Zinc stearate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 94.0000 %)
Type B	100.0000 % (> 99.9913 %)	100.0000 % (> 85.0000 %)
Type C	100.0000 % (> 99.9019 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
24018	24018	0.00	46.43
26123	26123	0.00	43.85

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

VALIDATION REPORT

IdentModule 2.9-2025-01

Validated substance/substance group	**Zinc sulfate heptahydrate**
Substance class	APIs & excipients, solid
Report date	06/03/2025
Report number	10006391-2025-03-06
Executing company	HiperScan GmbH Weißeritzstraße 3 01067 Dresden Germany

Relevant substance names

Zinc sulfate heptahydrate; Zinc sulphate heptahydrate; Zinci sulfas heptahydricus

Special notes

When selecting the *Zinc sulfate heptahydrate* substance/substance group, the following information is displayed to the user:

no information

Applicable documents

978-3-7692-8026-5	*European Pharmacopoeia 11th Edition, Basic Version 2022* [3]
Komm2.2.40	*Erfüllung von* Ph. Eur. 2.2.40 *durch* Apo-Ident [4]
AA004	*Erstellung und Validierung eines IdentModul-Updates*

Validation method

Validation is performed after every change to the chemometric model (also "database") in three steps:

1. The chemometric model is calculated from the calibration spectra using a *PCA algorithm*. The calibration spectra originate from the calibration samples of all substances in this class.
2. In the *chemometric model* generated, the distances between all separable substances are checked for compliance with the specified safety distances.
3. All spectra are presented to the generated chemometric model for evaluation. In three runs, the reference spectra (*Type A*), spectra from independent samples (*Type B*), and spectra from the field (*Type C*) are presented successively. Here, no single *false positive* result is permitted.

Finally, a report is generated from the validation run results and is archived together with the parameters of the model generation in audit-compliant manner.

Number of independent samples (batches) in calibration and validation

A sample is considered independent if no sample from the same batch has been included in the calibration of the chemometric model.

Substance/substance group	Type A	Type B	Type C
Zinc sulfate heptahydrate	2	2	13

Second-stage model

For differentiation of the substance/substance group *Zinc sulfate heptahydrate* the following second-stage model is used:

no second-stage model

Nearest chemometric neighbors (distance to the nearest foreign sample)

The following table lists the nearest chemometric neighbors of the substance/substance group *Zinc sulfate heptahydrate* in the substance class *APIs & excipients, solid*. For *Mahalanobis distances* M that do not meet the criterion $M \geq 9$, the differentiation is questioned. However, it is often possible that substances that the main model could not reliably separate from each other can be differentiated in a second-stage model.
A necessary condition for the output of a clear result is therefore: All substances in the second-stage model must have a distance $M \geq 9$ from each other. All remaining substances must reach $M \geq 9$ in the main model.
Where this is not achieved, an ambiguous result is shown as result which includes at least the two substances that are too close to each other as possible identities (substance group). Alternatively these substances can be excluded from the list of substances identifiable with Apo-Ident.

Substance	Distance in main model	Distance in second-stage model
Magnesium sulfate heptahydrate	24.75	–
Sodium cromoglicate	60.55	–

The list stops after the first substance with a *Mahalanobis distance* greater than 50. If the substance/substance group *Zinc sulfate heptahydrate* is separated from critical neighbours in a second-stage model, all the remaining substances in the second-stage model follow.

Calibration samples

Only spectra which have been recorded by *HiperScan GmbH* from traceable samples are used for the generation of the chemometric models. The following samples have been obtained from the substance/substance group *Zinc sulfate heptahydrate*:

Supplier	Substance	Batch	Sample ID	Spectra	Certificate
Euro OTC	Zinc sulfate heptahydrate	2206010	26554	40	20220624*
Euro OTC	Zinc sulfate heptahydrate	2206010	26554SI	20	20220624*
Euro OTC	Zinc sulfate heptahydrate	2210021	26555	40	20221122*
Euro OTC	Zinc sulfate heptahydrate	2210021	26555SI	20	20221122*

Validation samples

A total of 591 113 spectra were provided for validation. The results were evaluated separately according to the following sample categories:

Type A All calibration spectra.

- 120 spectra of 4 reference samples from the substance/substance group *Zinc sulfate heptahydrate*. These samples are listed above in the *calibration samples* section. The reference samples come from 2 different batches.

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

- 152 842 spectra from a total of 2840 batches from further 483 substances. These spectra were recorded by *HiperScan GmbH*. *Type A* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type A* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix A*. The samples in *Appendix A* were added for model generation not with the intention to have the model identify these substances, but with the intention to make the model reject them despite their similarity to substances identifiable.

Type B Spectra from independent samples not included in the database structure. Measurement is carried out by *HiperScan GmbH*.

Samples from batches of which no spectra have been included in the database structure are considered as independent samples. The number of batches from which independent samples supplied *Type B* spectra for validation is shown below, representing the number of independent *Type B* samples. Samples, of which some of the spectra have been included in the database structure and other spectra in the validation, are marked with a †. The following applies to the remaining unmarked samples: In the same batch, there was at least one additional sample (other sales container, other sample ID) from which reference spectra (*Type A*) were included in the database structure.

- 90 spectra of 2 reference samples from the substance/substance group *Zinc sulfate heptahydrate*.
- Among them are spectra of independent samples from 2 batches from which no spectra have been included in the database structure. They are sorted upwards in the following table and separated from the additional samples by a line.

Supplier	Substance	Batch	Sample ID	Spectra
Caelo	Zinc sulfate heptahydrate	23002587	27077	40
Euro OTC	Zinc sulfate heptahydrate	2107023	25788	50

- 201 994 spectra from a total of 4043 batches from further 838 substances. These spectra were recorded by *HiperScan GmbH*. *Type B* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type B* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix B*.

Type C Spectra of independent samples not included in the database structure. *Apo-Ident* customers carry out the measurements. *HiperScan GmbH* generally does not verify the information provided by the customer regarding manufacturer and batch number.

- 14 spectra from 10 *Apo-Ident* customers from 13 batches from the substance/substance group *Zinc sulfate heptahydrate*.
- Among them are spectra of independent samples from 13 batches from which no spectra have been included in the database structure. These are sorted upwards in the following table.

Supplier	Substance	Batch	Spectra
Caelo	Zinc sulfate heptahydrate	11095601	1
Caelo	Zinc sulfate heptahydrate	11095621	1
Caelo	Zinc sulfate heptahydrate	12257802	1
Caelo	Zinc sulfate heptahydrate	12257809	2
Caelo	Zinc sulfate heptahydrate	12257816	1
Caelo	Zinc sulfate heptahydrate	12257818	1
Caelo	Zinc sulfate heptahydrate	4012Q-02798	1
Caelo	Zinc sulfate heptahydrate	81554199	1
Euro OTC	Zinc sulfate heptahydrate	1105002-01	1
Euro OTC	Zinc sulfate heptahydrate	1201031-01	1
Euro OTC	Zinc sulfate heptahydrate	1201031-02	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Zinc sulfate heptahydrate	1201031-2	1
Euro OTC	Zinc sulfate heptahydrate	1309011_0	1

- 236 053 spectra from 1515 *Apo-Ident* customers from a total of 49 245 batches from a further 721 substances. These spectra were recorded by *Apo-Ident* customers. *Type C* samples are documented within this entire report. If the substance can be identified with this chemometric model, the samples are listed in the *Type C* section of each substance page. If the substance cannot be identified by this model, the samples are listed in *Appendix C*.

Validation results

The validation runs checked whether the substance/substance group *Zinc sulfate heptahydrate* can clearly be distinguished from all other substances using NIR spectroscopy with *Apo-Ident*. For this purpose, all relevant spectra of the various substances were compared with *Zinc sulfate heptahydrate* and it was evaluated how many matches (positive) and rejections (negative) were correct or incorrect. The following table breaks down the numbers of correct and incorrect results according to the expected result (*positive*/*negative*) and the validation spectrum type (*A*/*B*/*C*).

	False positive	True positive	False negative	True negative
Type A	0	120	0	152 842
Type B	0	90	0	201 994
Type C	0	14	0	236 053

The substance/substance group *Zinc sulfate heptahydrate* can be clearly distinguished from all other substances. In order to make these figures comparable, the weighted *true negative rate* (*specificity*) and the weighted *true positive rate* (*recognition rate*) are determined:

	Specificity	Recognition rate
Type A	100.0000 % (> 99.9909 %)	100.0000 % (> 95.0000 %)
Type B	100.0000 % (> 99.9912 %)	100.0000 % (> 93.3333 %)
Type C	100.0000 % (> 99.9008 %)	n/a (n/a)

In order to ensure that each substance is entered with the same weight irrespective of the number of spectra available, each spectrum is weighted with the reciprocal value of its number. (If several new spectra of a substance with a very distinctive spectrum are added, the values for *specificity* and *recognition rate* are safer, but are by no means idealised.)

In order to illustrate the impact of the number of spectra, a comparison is made in parentheses as to how the *specificity* or *recognition rate* would worsen if three additional incorrect results were to exist amongst the spectra (*Rule of Three* [10, 11]). The larger the number of spectra, the lower the deterioration if the three hypothetical *incorrect results* were added.
Where the number of spectra does not exceed 20, no *recognition rate* is provided.

Identity according to identity test using NIR spectroscopy

For each substance, a certificate of the correct identity is obtained from an independent GMP-certified test laboratory. If the identity of the sample can be provided using NIR on an independently tested reference sample, in the following table the *Mahalanobis distance* to the reference sample is specified as well as the *Mahalanobis distance* to the next non-identical substance:

Sample ID	Reference sample ID	Distance to reference sample	Distance to next foreign sample
26554	26554	0.00	75.81
26555	26555	0.00	44.10

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

The identity of a sample will be confirmed by NIR if the distance to the next foreign sample is at least 50 % greater than the distance to a reference sample whose identity has been established by laboratory testing. This criterion is always considered in the chemometric model, which contains all substances of the substance class, even if a second-stage dissolves a subgroup of similar substances, thereby increasing the distances between them. The samples confirmed by NIR support the statistical variance of the original reference substance, but cannot add new aspects or forms of the substance.

Appendix A: Additional calibration samples (*Type A*)

Substance spectra also enter the generation of the chemometric model which cannot be identified with this model. This serves the purpose that substances which the model is not supposed to recognise are safely rejected. The spectra of these samples are entered into the validation as *Type A*. They were recorded by *HiperScan GmbH*.

The samples originate from 264 batches. From these, 12 280 spectra were recorded. The calibration spectra of substances which can be identified with the model are listed respectively in the section *calibration samples* for the individual substances and do not appear again elsewhere in this list.

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Aloes, cape, powdered	12183008	40	20120802
Caelo	Aluminium potassium - sulfate dodecahydrate	12144605	40	from supplier
Caelo	Amphetamine sulfate	13344603	40	0814J-03361
Caelo	Amphetamine sulfate	16153902	40	2017A-03361
Caelo	Amphetamine sulfate	13344603	60	0814J-03361
Fagron	Amphetamine sulfate	13G08-N11	40	0814K-03361
Fagron	Amphetamine sulfate	15L01-B05-315291	60	1316Q-03361
Fagron	Amphetamine sulfate	13G08-N11	60	0814K-03361
Fagron	Amphetamine sulfate	15L01-B05-315291	60	1316Q-03361
Th. Geyer	Amphetamine sulfate	67002	40	0814I-03361
Th. Geyer	Amphetamine sulfate	067043	40	2017C-03361
Th. Geyer	Amphetamine sulfate	67002	60	0814I-03361
Flora Apot…	Amygdalin	13121802	40	1405619
Auropure L…	Amygdalin, bitter almond extract 98%	PA02099-17102131	40	from supplier
Safic-Alcan	Amygdalin, bitter almond extract 98%	BAE150902	60	from supplier
Safic-Alcan	Amygdalin, bitter almond extract 98%	BAE150902	60	from supplier
Caelo	Aniseed	13333903	40	20131018
Caelo	Aniseed, pounded	13357101	40	20131202
Klenk	Asparagus root, cut	6151B110304	40	1403480
Fagron	Barbital sodium	12F27-N02	40	0814I-07775
Fagron	Barbital sodium	14K14-B04-303353	60	1516I-07775
Fagron	Barbital sodium	12F27-N02	60	0814I-07775
Fagron	Barbital sodium	14K14-B04-303353	60	1516I-07775
Caelo	Bean shells	11030601	50	20110221
Euro OTC	Benfotiamine	2207006	40	20220729*
Euro OTC	Benfotiamine	2207006	20	20220729*
Caelo	Benzalkonium chloride	16171603	40	20160715
Merck KGaA	Benzoyl peroxide, hydrous	S7012241509	60	20130317
Sigma-Aldrich	Betamethasone acetate	LRAA8500	40	CRS
Sigma-Aldrich	Betamethasone sodium phosphate	MKBS9676V	40	CRS
Caelo	Bilberry fruit, dried	10265602	40	20101206
Klenk	Birch bark, cut	0561A121121	40	20121127
Caelo	Black cumin seed	161157	60	20160708
Klenk	Black mustard seed	7430A120813	40	AR-15-FG-001050-01
Caelo	Black mustard seed, powdered	12350204	80	1403711
Caelo	Blackcurrants	12272801	40	1403468
Caelo	Buprenorphine hydrochloride	12172908	40	0814I-07774
Caelo	Buprenorphine hydrochloride	16143001	40	2017A-07774
Euro OTC	Calcium carbonate	1611008-01	40	20161201
Flora Apot…	Calcium colamine phosphate	14384	40	from supplier

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Pharmorgana	Calcium colamine phosphate	1000200822	40	from supplier
Pharmorgana	Calcium colamine phosphate	1000210678	50	from supplier
Pharmorgana	Calcium colamine phosphate	1000230793	40	from supplier
Th. Geyer	Calcium colamine phosphate	33299	60	from supplier
Th. Geyer	Calcium colamine phosphate	66606	40	from supplier
Pharmorgana	Calcium L-aspartate trihydrate	1000230427	40	from supplier
Euro OTC	Calcium orotate dihydrate	1401006-01	40	1412540
Euro OTC	Calcium orotate dihydrate	1603003	40	20160329*
Euro OTC	Calcium orotate dihydrate	1603003	40	20180615*
Fagron	Calcium orotate dihydrate	12L04-N07	40	from supplier
Fagron	Calcium orotate dihydrate	13J23-N05	40	from supplier
Flora Apot...	Calcium orotate dihydrate	ORC00119	40	from supplier
Klenk	Calendula flower	1241B130321	40	20130408
Caelo	Calendula flower, cut	11187605	40	20110930
Caelo	Caraway fruit	11003217	40	20110209
Caelo	Caraway fruit, pounded	12116904	40	20120503
Caelo	Carnauba wax	170903	40	20170512*
Caelo	Carnauba wax	183330	40	20190114*
Caelo	Castoreum, powdered	12137409	40	1402590
Klenk	Celery fruit	7140A131122	60	20131204
Klenk	Celery root, cut	6091A110110	40	1410177
Caelo	Chicory root	11374504	40	20120112
Euro OTC	Cholecalciferol dry concentrate	1508032	60	20150901*
Euro OTC	Cholecalciferol dry concentrate	1608002	40	20160824*
Euro OTC	Cholecalciferol dry concentrate	2001007	40	20200316*
Pharmorgana	Chromium(III) orotate hexahydrate	760020	40	from supplier
Klenk	Clove, powdered (spice)	1264B141007	60	AR-15-FG-014858-01
Caelo	Cocaine hydrochloride	13259305	40	0814J-01278
Caelo	Cocaine hydrochloride	15224802	60	1316Q-01278
Caelo	Cocaine hydrochloride	15224802	60	1316Q-01278
Caelo	Cocaine hydrochloride	17003902	40	1917S-01278
Caelo	Cocaine hydrochloride	13259305	60	0814J-01278
Caelo	Cocaine hydrochloride	15224802	60	1316Q-01278
Caelo	Cocaine hydrochloride	15224802	60	1316Q-01278
Fagron	Cocaine hydrochloride	13I17-N02	40	0814I-01278
Fagron	Cocaine hydrochloride	16B11-B05-323386	40	1917Q-1278
Fagron	Cocaine hydrochloride	13I17-N02	60	0814I-01278
Th. Geyer	Cocaine hydrochloride	60145	40	0814K-01278
Th. Geyer	Cocaine hydrochloride	60145	60	0814K-01278
Caelo	Codeine phosphate hemihydrate	13071504	40	0814J-01279
Caelo	Codeine phosphate hemihydrate	15350703	60	1316R-01279
Caelo	Codeine phosphate hemihydrate	13071504	60	0814J-01279
Caelo	Codeine phosphate hemihydrate	15350703	60	1316R-01279
Fagron	Codeine phosphate hemihydrate	13C11-N10	40	0814I-01279

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Fagron	Codeine phosphate hemihydrate	15F09-B02-310520	60	1316Q-01279
Fagron	Codeine phosphate hemihydrate	16E17-B05-324109	40	2017A-01279
Fagron	Codeine phosphate hemihydrate	13C11-N10	60	0814I-01279
Fagron	Codeine phosphate hemihydrate	15F09-B02-310520	60	1316Q-01279
Th. Geyer	Codeine phosphate hemihydrate	67038	40	0814K-01279
Th. Geyer	Codeine phosphate hemihydrate	067054	40	2017D-01279
Th. Geyer	Codeine phosphate hemihydrate	67038	60	0814K-01279
Caelo	Colophony	12301410	60	AR-15-FG-016314-01
Caelo	Colophony	173014	40	20180102*
Caelo	Colophony	191664	40	20190701*
Klenk	Comfrey root	6244B130624	40	20130625
Klenk	Cumin, powdered	2824B121001	40	20121009
Fagron	Curcumin	CP2404071	40	20240410*
Fagron	Curcumin	CP2403046	40	20240320*
Euro OTC	Deoxycholic acid	1305051-01	40	from supplier
New Zealan…	Deoxycholic acid	0416720	40	from supplier
Sigma-Aldrich	Dexamethasone sodium phosphate	LRAC1690	40	CRS
Fagron	Dexamphetamine sulfate	13I23-N01	40	0814M-03582
Fagron	Dexamphetamine sulfate	15H06-B04-313862	60	1316Q-03582
Fagron	Dexamphetamine sulfate	16D20-B01-321049	40	2017B-03582
Fagron	Dexamphetamine sulfate	13I23-N01	60	0814M-03582
Sigma-Aldrich	Diclofenac potassium	D1039990	40	CRS
Caelo	Dihydrocodeine hydrogen tartrate	13267601	40	0914A-03065
Caelo	Dihydrocodeine hydrogen tartrate	12142506	40	0914B-03065
Caelo	Dihydrocodeine hydrogen tartrate	15295901	60	1316Q-03065
Caelo	Dihydrocodeine hydrogen tartrate	13267601	60	0914A-03065
Caelo	Dihydrocodeine hydrogen tartrate	12142506	60	0914B-03065
Caelo	Dihydrocodeine hydrogen tartrate	15295901	60	1316Q-03065
Fagron	Dihydrocodeine hydrogen tartrate	13H19-N03	40	0914C-03065
Fagron	Dihydrocodeine hydrogen tartrate	14K26-B04-306298	60	1516I-03065
Fagron	Dihydrocodeine hydrogen tartrate	15F18-B07-323388	40	2017A-03065
Fagron	Dihydrocodeine hydrogen tartrate	13H19-N03	60	0914C-03065
Th. Geyer	Dihydrocodeine hydrogen tartrate	67035	40	0914D-03065
Th. Geyer	Dihydrocodeine hydrogen tartrate	067052	40	2017D-03065
Th. Geyer	Dihydrocodeine hydrogen tartrate	67035	60	0914D-03065
Caelo	Dill herb, cut	11295103	40	20111103
Safic-Alcan	Dimercaptosuccinic acid	20170210	40	from supplier
Fagron	Diosmin	DSM240602	40	20241031*
Fagron	Diosmin	DSM240401	40	20241031*

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Fagron	Econazole nitrate	12H08-N02	40	1312442
Fagron	Econazole nitrate	11F09-N16	40	20110606
Fagron	Econazole nitrate	12I06-B40-306925	40	AR-16-FG-011359-01
Fagron	Econazole nitrate	14G22-B07-327805	40	20140804
Yino Pharma	Enoxaparin sodium	YN010232209001	40	20230524*
Yino Pharma	Enoxaparin sodium	YN010232210002	40	20230524*
Yino Pharma	Enoxaparin sodium	YN010232209001	20	20230524*
Yino Pharma	Enoxaparin sodium	YN010232210002	20	20230524*
EDQM	Erythromycin lactobionate	1.0	40	CRS
Caelo	Eucalyptus leaf	11307706	40	20111111
Fagron	Fentanyl citrate	13G30-N06	40	0814M-07678
Fagron	Fentanyl citrate	15F18-B01-525098	60	1316R-03686
Fagron	Fentanyl citrate	15F18-B01-525166	60	1316Q-03686
Fagron	Fentanyl citrate	13G30-N06	60	0814M-07678
Fagron	Fentanyl citrate	15F18-B01-525098	60	1316R-03686
Fagron	Fentanyl citrate	15F18-B01-525166	60	1316Q-03686
EDQM	Fenticonazole nitrate	1.3	40	CRS
Euro OTC	Fexofenadine hydrochloride	2310018	30	20240222*
Flora Apot…	Frankincense	JR-RX20230716CG	40	not required
Caelo	Ginger	12180601	40	20120730
Caelo	Ginger	11325715	40	20111205
Klenk	Ginger, peeled, powdered	6954B160429	60	1704440
Fagron	Glucosamine sulfate potassium chloride	TSM-K-2404002	40	20240928*
Fagron	Glucosamine sulfate potassium chloride	TSM-K-2404001	40	20240928*
Flora Apot…	Glycyrrhizic acid	10588	40	from supplier
Euro OTC	Griffonia seed extract	1205027	40	from supplier
Euro OTC	Griffonia seed extract	1705007	40	20170601*
Euro OTC	Griffonia seed extract	1905017	40	20190709*
Pharmorgana	Griffonia seed extract	1000200297	40	from supplier
Caelo	Hay flowers	12317104	40	20121122
Klenk	Hay flowers	1400A130304	40	20130403
Bombastus	Hop strobile	23003461	30	20230809
Fagron	Hydrocortisone butyrate	15J12-B03-322394	40	20151028
Caelo	Hydromorphone hydrochloride	13267702	40	0914A-01334
Caelo	Hydromorphone hydrochloride	15393602	60	1516J-01334
Caelo	Hydromorphone hydrochloride	13267702	60	0914A-01334
Caelo	Hydromorphone hydrochloride	15393602	60	1516J-01334
Fagron	Hydromorphone hydrochloride	13E16-N02	40	0914B-01334
Fagron	Hydromorphone hydrochloride	13I25-N05	60	1516I-01334
Fagron	Hydromorphone hydrochloride	15L08-B08-316877	40	1917Q-01334
Fagron	Hydromorphone hydrochloride	13E16-N02	60	0914B-01334
Fagron	Hydromorphone hydrochloride	13I25-N05	60	1516I-01334
Fagron	Hydroxytryptophan (L-5-)	22A17-B03-226102	40	240603342
Caelo	Iceland moss	12187106	40	1403493
Caelo	Iceland moss	13350803	40	20131114
Caelo	Ispaghula husks	13238005	40	20130816
Caelo	Juniper berry, pounded	13367302	40	20131122
Caelo	Kap-Aloe	11048808	40	20110315
Caelo	Kelp, cut	13230805	40	AR-15-FG-007678-01

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Kelp, cut	15418801	60	AR-17-FG-007505-01
Dr. Behr	L-Carnitine hydrochloride	WE11030091	60	from supplier
Dr. Behr	L-Carnitine tartrate	WE11060069	40	from supplier
Dr. Behr	L-Carnitine tartrate	WE15080050	60	from supplier
Euro OTC	L-Carnitine tartrate	1302017-01	40	from supplier
Fagron	L-Carnitine tartrate	10100220240309	40	20260228*
Flora Apot...	Levamisole hydrochloride	LV17203	40	from supplier
Caelo	Linseed	12186902	60	pending
Caelo	Linseed	13412801	40	20140113
Galke	Liqourice root, peeled	22728	40	from supplier
Fagron	Losartan potassium	D5440-24-006	40	20240410*
Caelo	Magnesium carbonate, heavy	182282	40	20180906*
Caelo	Marshmallow root	11101905	40	20110406
Caelo	Marshmallow root	13214804	40	20130806
Caelo	Matricaria flower	12337605	40	20121122
Caelo	Mellisa leaf	13214713	40	20130806
Caelo	Methadone hydrochloride	12344818	40	0914E-02949
Caelo	Methadone hydrochloride	15244715	60	1516A-02949
Caelo	Methadone hydrochloride	12344818	60	0914E-02949
Caelo	Methadone hydrochloride	15244715	60	1516A-02949
Fagron	Methadone hydrochloride	13J24-B06	40	0914F-02949
Fagron	Methadone hydrochloride	15E29-B02-313098	60	1516B-02949
Fagron	Methadone hydrochloride	16F24-B02-323183	40	1917Q-02949
Fagron	Methadone hydrochloride	13J24-B06	60	0914F-02949
Fagron	Methadone hydrochloride	15E29-B02-313098	60	1516B-02949
Th. Geyer	Methadone hydrochloride	67033	40	0914G-02949
Th. Geyer	Methadone hydrochloride	67047	40	0914H-02949
Th. Geyer	Methadone hydrochloride	67033	60	0914G-02949
Th. Geyer	Methadone hydrochloride	67047	60	0914H-02949
Flora Apot...	Mg-Ca-K colamine phosphate	1000190952	40	from supplier
Th. Geyer	Mg-Ca-K colamine phosphate	36985	60	from supplier
Th. Geyer	Mg-Ca-K colamine phosphate	46816	40	from supplier
Th. Geyer	Mg-Ca-K colamine phosphate	80919	40	from supplier
Caelo	Midazolam hydrochloride	12215811	40	0914E-03538
Caelo	Midazolam hydrochloride	15224602	60	1516B-03538
Caelo	Midazolam hydrochloride	12215811	60	0914E-03538
Caelo	Midazolam hydrochloride	15224602	60	1516B-03538
Fagron	Midazolam hydrochloride	13E22-N09	40	0914F-03538
Fagron	Midazolam hydrochloride	14L23-B04-300245	60	1516A-03538
Fagron	Midazolam hydrochloride	15H04-B03-314396	40	1917R-03538
Fagron	Midazolam hydrochloride	16C14-B12-332469	40	0718E-03538
Fagron	Midazolam hydrochloride	13E22-N09	60	0914F-03538
Fagron	Midazolam hydrochloride	14L23-B04-300245	60	1516A-03538
Fagron	Midazolam hydrochloride	16C14-B12-332469	40	0718E-03538
Fagron	Minoxidil sulfate	01801022407017	40	20241230*
Fagron	Minoxidil sulfate	01801022405015	40	20240930*
Caelo	Mistletoe	11294003	30	20111027
Caelo	Morphine hydrochloride	13125207	40	0914E-01879
Caelo	Morphine hydrochloride	13349505	40	0914F-01879
Caelo	Morphine hydrochloride	15439404	60	1416R-01879
Caelo	Morphine hydrochloride	16184605	40	1917S-01879
Caelo	Morphine hydrochloride	13125207	60	0914E-01879
Caelo	Morphine hydrochloride	13349505	60	0914F-01879
Caelo	Morphine hydrochloride	15439404	60	1416R-01879
Fagron	Morphine hydrochloride	13G08-N04	40	0914G-01879

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Fagron	Morphine hydrochloride	15I09-B08-312694	60	1416Q-01879
Fagron	Morphine hydrochloride	13G08-N04	60	0914G-01879
Fagron	Morphine hydrochloride	15I09-B08-312694	60	1416Q-01879
Th. Geyer	Morphine hydrochloride	67036	40	0914H-01879
Th. Geyer	Morphine hydrochloride	67036	60	0914H-01879
Caelo	Myrrh	11277111	60	1403081
Caelo	Myrrh	13108701	40	AR-15-FG-000946-01
Klenk	Nutmeg, powdered (spice)	7325A160405	60	9888
Fagron	Orlistat	6012307004-01	40	20240523*
Fagron	Orlistat	6012307003-02	40	20240526*
Caelo	Orris root	11026705	40	20110221
Klenk	Parsley seed	7370A130909	40	1407600
Caelo	Pepper	11193905	40	20110727
Caelo	Peppermint leaf	11347607	40	20111220
Caelo	Phenobarbital	12173202	40	0914E-01040
Caelo	Phenobarbital	12173202	60	0914E-01040
Fagron	Phenobarbital	15G07-B06-311718	60	1416Q-01040
Fagron	Phenobarbital	15G07-B06-311718	60	1416Q-01040
Th. Geyer	Phenobarbital	67045	40	0914F-01040
Th. Geyer	Phenobarbital	067056	40	2017A-01040
Th. Geyer	Phenobarbital	67045	60	0914F-01040
Euro OTC	Potassium orotate	1203038V-02	60	from supplier
Euro OTC	Potassium orotate	1203038V-02	40	9757
Flora Apot…	Potassium orotate	ORK00117	40	from supplier
Fagron	Pullulan	24H27-B078	40	20240916*
Caelo	Rhubarb	11057818	40	20110314
Caelo	Rosemary leaf	11193408	40	20110728
Caelo	Siam benzoin	12321312	40	pending
Caelo	Siam benzoin	12321314	40	20121031
Pharmorgana	Sodium dichloroacetate	1000150016	40	from supplier
Caelo	Star anise	11314104	30	20111121
Fagron	Sunset yellow	13I05_N04	40	20130903
Klenk	Tormentil	6911B141114	60	AR-15-FG-014020-01
EDQM	Triamcinolone hexacetonide	3.0	40	CRS
Caelo	White mustard seed	12361002	40	1403473
Caelo	White mustard seed, powdered	12349601	60	1403281
Caelo	White mustard seed, powdered	12375705	40	20130110

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Appendix B: Additional validation samples (*Type B*)

It is necessary that spectra also enter the validation which cannot be identified with this model. In this manner, it is verified that the model also rejects unknown substances. The spectra for these samples were recorded by *HiperScan GmbH*. They are allocated to the *Type B*. They also include the calibration spectra for other models.

The samples originate from 1246 batches. From these 50 011 spectra were recorded. The spectra recorded on independent samples of substances which can be identified with the model are listed respectively in the section *Type B* for the individual substances and do not appear again elsewhere in this list.

Supplier	Substance	Batch	Spectra	Certificate
Fagron	(R,S)-epinephrine hydrochloride	12H08-N03	40	no certificate available
Fagron	(R,S)-epinephrine hydrochloride	14A22-B05-291560	60	no certificate available
Fagron	(R,S)-epinephrine hydrochloride	16H23-B98-325052	40	20160913
Fagron	5-fluorouracil	13F19-N03	40	1402308
Fagron	5-fluorouracil	13F19-N03	60	1608169
Fagron	5-fluorouracil	16D01-U05/3-327376	40	20161117
Fagron	8-quinolinol sulfate monohydrate	12H21-N08	40	20120831
Fagron	Acetyl-L-carnitine hydrochloride	24H27-B070	40	20240923*
Fagron	Acetyl-L-carnitine hydrochloride	24H27-B070	20	20240923*
Caelo	Acorus root	12076404	40	20120328
Caelo	Acorus root, peeled	12239001	40	20120905
Caelo	Acorus root, peeled	12295902	40	20121025
Caelo	Agarikon	11024502	40	20110125
Caelo	Agarikon	13130602	48	1405003
Caelo	Agarikon	14190702	60	20140730
Caelo	Agarikon	14190706	60	20140730
Klenk	Agarikon	1061A120312	40	pending
Caelo	Agnus castus fruit	12274003	40	1501649
Caelo	Agnus castus fruit	13193401	40	AR-15-FG-006453-01
Caelo	Agnus castus fruit	15318705	60	pending
Caelo	Agrimony	10325505	45	20101221
Caelo	Agrimony	11374004	40	20120125
Caelo	Alchemilla	12153306	40	20120618
Caelo	Alchemilla alpina herb, cut	12147201	40	20120608
Caelo	Allspice, powdered (spice)	12042703	40	from supplier
Caelo	Almonds, bitter, whole	13220401	40	1406296
Caelo	Aloes, cape, powdered	11132115	40	1404400
Caelo	Aloes, cape, powdered	11132115	40	20110520
Caelo	Aluminium oxide, hydrated	12163019	40	20120621
Caelo	Aluminium oxide, hydrated	13119121	40	20130503
Sigma-Aldrich	Aluminum hydroxide hydrate	102465140	40	not required
Sigma-Aldrich	Aluminum sodium silicate	102527683	40	not required
Fagron	Amiodarone hydrochloride	18J26-B01-368910	40	20200429
Fagron	Amiodarone hydrochloride	18J26-B01-368910	20	20200429
Sigma-Aldrich	Ammonium bromide	0000097635	40	not required
Caelo	Ammonium chloride	12356101	40	20121206
Euro OTC	Ammonium chloride	1209013-01	40	20120928
Caelo	Amphetamine sulfate	18186907	40	1919M-03361
Caelo	Amphetamine sulfate	16153902	40	2017A-03361
Caelo	Amphetamine sulfate	18186907	40	1919M-03361
Fagron	Amphetamine sulfate	16A29-B03-324577	40	2017B-03361

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Fagron	Amphetamine sulfate	16A29-B03-324577	40	2017B-03361
Th. Geyer	Amphetamine sulfate	067043	40	2017C-03361
abcr GmbH	Amygdalin	1310927	40	from supplier
abcr GmbH	Amygdalin	1310579	40	from supplier
Auropure L...	Amygdalin, bitter almond extract 98%	PA02099-160822	30	from supplier
Caelo	Angelica root	12168701	40	pending
Caelo	Angelica root	12080404	40	1403053
Caelo	Angelica root	12080409	40	20120322
Klenk	Angelica root	6085B120614	40	20120621
Klenk	Angelica root	6085B120614	60	1509356
Caelo	Aniseed	11370301	40	20120117
Klenk	Aniseed	2700A140129	60	20140926
Klenk	Aniseed	2700A160511	60	1708049
Caelo	Aniseed, pounded	12111301	40	20120420
Caelo	Aniseed, powdered	11306203	40	20111110
Caelo	Apple, cut	11229807	60	from supplier
Caelo	Arnica flower	11285702	40	20111118
Caelo	Arnica flower	11259801	40	20110923
Caelo	Artichoke leaf	12173302	40	20120706
Caelo	Artichoke leaf	13310707	40	20130930
Caelo	Artificial thermal salt a	181633	40	20180621*
Klenk	Ash bark, cut	0871B110127	60	20110128
Caelo	Ash leaf, cut	11031303	40	20110224
Caelo	Asparagus root, cut	10299010	40	pending
Fagron	Aspartame	21I21-B07-213840	40	20211216
Fagron	Aspartame	21I21-B07-213840	20	20211216
Fagron	Azithromycin	20F22-F01-372739	50	20200813
Fagron	Azithromycin	24C14-B02-231046	40	20240507
Fagron	Azithromycin	24C14-B02-231046	20	20240507
Caelo	Barberries	11058309	40	pending
Caelo	Barberries	12217109	60	pending
Caelo	Barberries	14057312	60	1508391
Caelo	Barberry root bark, cut	12112601	40	20120430
Fagron	Barbital sodium	15L07-B02-324539	40	2017A-07775
Fagron	Barbital sodium	15L07-B02-324539	40	2017A-07775
Caelo	Barium sulfate	171113	40	20170509*
Caelo	Basil, rubbed	12066404	50	20120321
Caelo	Bearberry leaf	12186502	40	20120705
Fagron	Benfotiamine	NL/BA/0152324	40	20240801*
Fagron	Benfotiamine	NL/BA/0152324	20	20240801*
Caelo	Bentonite	12237603	40	20120810
Euro OTC	Betaine hydrochloride	2201015	40	not required
Euro OTC	Betaine hydrochloride	2309009	40	20231027*
Euro OTC	Betaine hydrochloride	2201015	10	not required
Euro OTC	Betaine hydrochloride	2309009	20	20231027*
Fagron	Betaine hydrochloride	13H13-N02	40	1402684
Fagron	Betaine hydrochloride	BH20240119	40	20270117*
Fagron	Betaine hydrochloride	BH20240119	20	20270117*
Gatt-Koller	Betaine hydrochloride	23J02134	40	20231121
Gatt-Koller	Betaine hydrochloride	23J02134	20	20231121
Caelo	Betony herb, cut	12007205	40	20120118
Caelo	Betony herb, cut	12007205	60	20120118
Caelo	Bilberry leaf	12140206	40	20120605
Caelo	Birch leaf	12193105	40	20120710
Caelo	Bismuth subnitrate, heavy	181942	40	20181010*
Fagron	Bisoprolol fumarate	24I18-B04-003143	40	20241003
Fagron	Bisoprolol fumarate	24I18-B04-003143	20	20241003
Caelo	Bitter-Orange flower (petals)	12266605	40	20120907

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Bitter-Orange flower (petals)	12266703	40	20120907
Caelo	Bitter-Orange peel	12067405	40	20120327
Caelo	Black cohosh	10281112	40	20101118
Caelo	Black cohosh	13237901	40	pending
Caelo	Black cohosh	13237903	40	20130812
Caelo	Black cumin seed	11233503	40	1403495
Caelo	Black mustard seed	12189303	40	1403472
Caelo	Black mustard seed	15120405	60	AR-17-FG-007964-01
Caelo	Black mustard seed	23000940006	30	20230523
Caelo	Black mustard seed, powdered	13358304	40	pending
Caelo	Black mustard seed, powdered	16051807	60	9887
Klenk	Black mustard seed, powdered	7434A120712	40	AR-15-FG-006711-01
Caelo	Blackberry leaf	11030707	40	20110303
Galke	Blackberry leaf	18060	40	20111021
Caelo	Blackcurrant leaf, cut	12168804	40	20120711
Caelo	Blackcurrants	14212502	60	20140829
Caelo	Blackcurrants	14212509	60	20140829
Caelo	Blackthorn flower	12178101	40	20120718
Caelo	Blessed thistle, cut	12038203	40	20120306
Caelo	Blue bottle flower	10291105	40	pending
Caelo	Blue bottle flower	13241902	60	AR-15-FG-005838-01
Caelo	Bogbean leaf, cut	12226101	40	20120809
Caelo	Boldo leaf	13367904	40	20131122
Galke	Boldo leaf	19855	40	20120727
Klenk	Boldo leaf	1911A100714	40	20111214
Caelo	Borage herb, cut	11206712	40	20110822
Roth	Brilliant blue R 250 (C.I.42660)	314217301	60	from supplier
Fagron	Bromelain	14F20-B03295501	40	pending
Fagron	Bromelain	14F20-B03295501	60	20140701
Sigma-Aldrich	Bromelain	BCBM1589V	40	from supplier
EDQM	Bromhexine hydrochloride	5.0	40	CRS
Caelo	Bucho leaf	12034903	40	20120221
Klenk	Buckwheat seed	7510A111011	40	from supplier
Klenk	Buckwheat seed	7510A111011	60	pending
Caelo	Buprenorphine hydrochloride	16143001	40	0718E-07774
Caelo	Buprenorphine hydrochloride	16143001	40	1919M-07774
Caelo	Buprenorphine hydrochloride	12172908	60	0814I-07774
Caelo	Buprenorphine hydrochloride	16143001	40	2017A-07774
Caelo	Buprenorphine hydrochloride	16143001	40	0718E-07774
Caelo	Buprenorphine hydrochloride	16143001	40	1919M-07774
Caelo	Burdock root	11100801	40	20110523
Caelo	Burnet root	12027410	40	20120206
Caelo	Burnet root	12027407	40	20120206
Caelo	Burnet root	12024406	40	20120206
Gatt-Koller	Caffeine-sodium benzoate	22J00803	40	20220530
Gatt-Koller	Caffeine-sodium benzoate	23J01215	40	20230803
Gatt-Koller	Caffeine-sodium benzoate	22J00803	20	20220530
Gatt-Koller	Caffeine-sodium benzoate	23J01215	20	20230803
Caelo	Calcium chloride dihydrate	182411	35	20181022*

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Calcium chloride dihydrate	23001613	40	20230717*
VWR Intern...	Calcium chloride hexahydrate	22K294102	40	not required
Th. Geyer	Calcium colamine phosphate	36986	40	from supplier
Euro OTC	Calcium orotate dihydrate	1009035-01	40	20101019
Euro OTC	Calcium orotate dihydrate	1411003	40	20160331*
Fagron	Calcium orotate dihydrate	16F13-B04-324144	40	20161108
Caelo	Calcium oxide	182244	39	20181106*
Caelo	Calcium sulfate dihydrate	163363	40	20161214*
Caelo	Calcium sulfate hemihydrate	153451	30	20151103*
Bombastus	Calendula flower	24002342	30	20240528
Caelo	Calendula flower	11221404	40	20110930
Caelo	Calendula flower	22003249004	30	20221214
Caelo	Campeche wood	11074105	40	from supplier
HiperScan	Cannabidiolic acid	19802	30	20240730
bubatzbros.de	Cannabis flower	BBCD11-092023	30	00080
bubatzbros.de	Cannabis flower	BBMK11-092023	30	00081
Cansativa	Cannabis flower	06051825121-2-P2	30	00001
Cansativa	Cannabis flower	ICC230402	30	00002
Cansativa	Cannabis flower	ICC230503	30	00003
Cansativa	Cannabis flower	WES230301	30	00004
Cansativa	Cannabis flower	GG4230303Y	30	00005
Cansativa	Cannabis flower	ZRP230101	30	00006
Cansativa	Cannabis flower	28202	30	00007
Cansativa	Cannabis flower	13302	30	00008
Cansativa	Cannabis flower	06051822121-3-P1	30	00009
Cansativa	Cannabis flower	02209916122-1-P3	30	00010
Cansativa	Cannabis flower	C038	30	00011
Cansativa	Cannabis flower	C086	30	00012
Cansativa	Cannabis flower	C082	30	00013
Cansativa	Cannabis flower	BKS2290001-1R1-6	30	00014
Cansativa	Cannabis flower	22K07FP23A18	30	00015
Cansativa	Cannabis flower	22K28FB23C15	30	00016
Cansativa	Cannabis flower	22I05EY22K30	30	00017
Cansativa	Cannabis flower	22H08FR22I28	30	00018
Cansativa	Cannabis flower	AKH2311001-1R1-6	30	00019
Cansativa	Cannabis flower	S87B2056CA-2R3-6	30	00020
Cansativa	Cannabis flower	91K2137CA-1R2-6	30	00021
Cansativa	Cannabis flower	LSK2216001-1R2-6	30	00022
Cansativa	Cannabis flower	22TC06HB010102	30	00023
Cansativa	Cannabis flower	22GS02SI010202	30	00024
Cansativa	Cannabis flower	C091	30	00025
Cansativa	Cannabis flower	D016	30	00026
Cansativa	Cannabis flower	D013	30	00027
Cansativa	Cannabis flower	D032	30	00028
Cansativa	Cannabis flower	030122LS-T22/10	30	00029
Cansativa	Cannabis flower	P22057FT	30	00030
Cansativa	Cannabis flower	P22055FT	30	00031
Cansativa	Cannabis flower	P22050FT-A	30	00032
Cansativa	Cannabis flower	02209951121-2-P1	30	00033
Cansativa	Cannabis flower	02209910122-3-P1	30	00034
Cansativa	Cannabis flower	CMNG23FSRE032877	30	00035
Cansativa	Cannabis flower	02209912122-1-P3	30	00036
Cansativa	Cannabis flower	22GS12WLC010105	30	00037
Cansativa	Cannabis flower	22GS12MG010102	30	00038
Cansativa	Cannabis flower	22GS15BB010202	30	00039
Cansativa	Cannabis flower	22GS02MK020102	30	00040
Cansativa	Cannabis flower	2203GG010402	30	00041

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Cansativa	Cannabis flower	21GS11HB040104	30	00042
Cansativa	Cannabis flower	2203PD010105	30	00043
Cansativa	Cannabis flower	22TC08HB010103	30	00044
Cansativa	Cannabis flower	21GS06ISS040102	30	00045
Cansativa	Cannabis flower	21GS06ISS040102	30	00046
Cansativa	Cannabis flower	21GS06MG030106	30	00047
Cansativa	Cannabis flower	22GS10PPS010102	30	00048
Cansativa	Cannabis flower	22TC05SI010102	30	00049
Cansativa	Cannabis flower	2GS02BB010105	30	00050
Cansativa	Cannabis flower	22GS02GWO010103	30	00051
Cansativa	Cannabis flower	22TC07PK010103	30	00052
Cansativa	Cannabis flower	C060	30	00053
Cansativa	Cannabis flower	02209920122-1-P1	30	00054
Cansativa	Cannabis flower	02209913122-1-P1	30	00055
Cansativa	Cannabis flower	P22058FT	30	00056
Cansativa	Cannabis flower	22GS12WLC010105	30	00057
Cansativa	Cannabis flower	TRP230603	30	00058
Cansativa	Cannabis flower	GG4230506	30	00059
Cansativa	Cannabis flower	28302	30	00060
Cansativa	Cannabis flower	28303	30	00061
Cansativa	Cannabis flower	2306605	30	00062
Cansativa	Cannabis flower	D043	30	00063
Cansativa	Cannabis flower	VA0163-2301	30	00064
Cansativa	Cannabis flower	06051821121-1-P1	30	00065
Cansativa	Cannabis flower	ICC230503	30	00089
Cansativa	Cannabis flower	WES230301	30	00090
Cansativa	Cannabis flower	ZRP230101	30	00091
Cansativa	Cannabis flower	28202	30	00092
Cansativa	Cannabis flower	C038	29	00093
Cansativa	Cannabis flower	S87B2056CA-2R3-6	30	00097
Cansativa	Cannabis flower	LSK2216001-1R2-6	30	00098
Cansativa	Cannabis flower	D013	30	00099
Cansativa	Cannabis flower	D032	31	00100
Cansativa	Cannabis flower	P22057FT	30	00101
Cansativa	Cannabis flower	P22050FT-A	30	00102
Cansativa	Cannabis flower	22GS12WLC010105	30	00103
Cansativa	Cannabis flower	02209913122-1-P1	30	00104
Cansativa	Cannabis flower	P22058FT	30	00105
Cansativa	Cannabis flower	22GS12WLC010105	30	00106
Cansativa	Cannabis flower	TRP230603	30	00107
Cansativa	Cannabis flower	28302	30	00108
Cansativa	Cannabis flower	28303	30	00109
Cansativa	Cannabis flower	2306605	20	00110
Cansativa	Cannabis flower	D043	30	00111
Cansativa	Cannabis flower	C038	31	00112
Cansativa	Cannabis flower	HSK2145CA-3R2-6	30	00116
Cansativa	Cannabis flower	LSK2216001-1R2-6	30	00117
Cansativa	Cannabis flower	D032	30	00118
Cansativa	Cannabis flower	P22057FT	30	00119
Cansativa	Cannabis flower	P22050FT-A	30	00120
Cansativa	Cannabis flower	22GS12WLC010105	30	00121
Cansativa	Cannabis flower	P22058FT	30	00122
Cansativa	Cannabis flower	28302	30	00123
Cansativa	Cannabis flower	2306605	30	00124
Cansativa	Cannabis flower	D043	30	00125
Cansativa	Cannabis flower	06051825121-2-P2	30	00126
Cansativa	Cannabis flower	06051822121-3-P1	30	00127
Cansativa	Cannabis flower	22GS12MG010102	30	00128
Cansativa	Cannabis flower	22GS15BB010202	30	00129
Cansativa	Cannabis flower	D013	30	00130

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Cansativa	Cannabis flower	22GS12WLC010105	40	00131
CBD NOL	Cannabis flower	CNRK8-092023	30	00132
CBD NOL	Cannabis flower	CNSLH5-092023	30	00133
CBD NOL	Cannabis flower	CNC5-092023	30	00134
CBD NOL	Cannabis flower	CNPK6-092023	30	00135
CBD NOL	Cannabis flower	CNAH6-092023	30	00136
CBD NOL	Cannabis flower	CNPE6-092023	30	00137
CBD NOL	Cannabis flower	CNBB0-092023	30	00138
CBD NOL	Cannabis flower	CNBA10-092023	30	00139
Hanfgarten.at	Cannabis flower	HCB000020	30	00082
Hanfgarten.at	Cannabis flower	HCB000019	37	00083
Hanfgarten.at	Cannabis flower	HCB000021	30	00084
Hanfgarten.at	Cannabis flower	HCB000014	31	00085
Hanfgarten.at	Cannabis flower	HCB000040	31	00086
Hanfgarten.at	Cannabis flower	HCB000015	40	00087
Hanfgarten.at	Cannabis flower	HCB000046	30	00088
happy420.de	Cannabis flower	100000318	30	00066
happy420.de	Cannabis flower	100000019	30	00067
happy420.de	Cannabis flower	100000814	30	00068
happy420.de	Cannabis flower	100000017	30	00069
happy420.de	Cannabis flower	100000024	30	00070
happy420.de	Cannabis flower	100000365	30	00071
happy420.de	Cannabis flower	100000167	30	00072
justbob	Cannabis flower	ES239230223	30	00073
justbob	Cannabis flower	ES259061222	30	00074
justbob	Cannabis flower	ES326090523	30	00075
Luckyhemp.de	Cannabis flower	BN-0033-03	30	00076
Luckyhemp.de	Cannabis flower	BN-0009-03	30	00077
Luckyhemp.de	Cannabis flower	BN-0003-03	30	00078
Luckyhemp.de	Cannabis flower	BN-0041-03	30	00079
Bombastus	Caraway fruit	23004707	30	20231023
Caelo	Caraway fruit	13397104	40	AR-15-FG-001526-01
Caelo	Caraway fruit	13397104	60	AR-15-FG-001527-01
Caelo	Caraway fruit	13306006	60	AR-16-FG-000540-03
Caelo	Caraway fruit	15097115	60	AR-17-FG-006649-01
Caelo	Caraway fruit	22003284004	30	20230228
Caelo	Caraway fruit, pounded	13367101	40	20130503
Caelo	Caraway fruit, pounded	14358801	60	AR-15-FG-014914-01
Caelo	Caraway fruit, pounded	16073201	60	AR-17-FG-006648-01
Caelo	Carbachol	11150302	31	1401147
Fagron	Carbidopa monohydrate	23A26-B05-226465	40	20230330
Fagron	Carbidopa monohydrate	23I12-B04-236349	40	20231108
Fagron	Carbidopa monohydrate	23A26-B05-226465	20	20230330
Fagron	Carbidopa monohydrate	23I12-B04-236349	20	20231108
Caelo	Cardamom fruit	11309107	40	20111111
Caelo	Cardamom fruit	13260504	40	20130906
Klenk	Cardamom, excorticated, powdered (spice)	2765A130524	60	AR-15-FG-015285-01
Lycored corp.	Caromix	CMX-LLCV-011401	40	20140131
Fagron	Carvedilol	22B21-F02-383500	40	20221111
Fagron	Carvedilol	22B21-F02-383500	20	20221111
Caelo	Castoreum, powdered	13410403	40	20131231
Caelo	Castoreum, powdered	13410403	40	20131231
Euro OTC	Cefaclor monohydrate	2311015	40	20240110*
Euro OTC	Cefaclor monohydrate	2310002	40	20240110*
Euro OTC	Cefaclor monohydrate	2311015	20	20240110*
Euro OTC	Cefaclor monohydrate	2310002	20	20240110*
Klenk	Celery fruit	7140A130625	40	1405177
Klenk	Celery fruit	7140A230110-01	30	20230214
Caelo	Celery root, cut	10270002	40	20101006

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Centaury	11097602	40	20110428
Euro OTC	Cetirizine dihydrochloride	2210014	40	20230112*
Euro OTC	Cetirizine dihydrochloride	2210014	20	20230112*
Fagron	Cetirizine dihydrochloride	23C08-B01-227628	40	20230422
Fagron	Cetirizine dihydrochloride	23C08-B01-227628	20	20230422
Caelo	Charcoal, activated	181885	40	20180813*
Klenk	Chervil, rubbed	3721A100329	40	20111128
Caelo	Chickweed, cut	13040502	40	1403482
Caelo	Chickweed, cut	13254411	40	1412550
Caelo	Chicory herb	12034303	60	20120228
Caelo	Chicory herb	12354302	100	20121211
Fagron	Chlorhexidine dihydrochloride	14A09-B03-290724	40	AR-15-FG-012308-01
Fagron	Chlorhexidine dihydrochloride	16C11-B02-324203	40	20160412
Fagron	Chlorhexidine dihydrochloride	16C11-B02-322510	40	20160412
Fagron	Chlorhexidine dihydrochloride	16C11-B02-329881	40	20160412
Fagron	Chlorobutanol hemihydrate	14A06-B31-290310	60	1412458
Fagron	Chloroquine phosphate	24002C3RJ	40	20240124*
Fagron	Chloroquine phosphate	24002C3RJ	20	20240124*
Euro OTC	Cholecalciferol dry concentrate	1210051-01	40	1403341
Euro OTC	Cholecalciferol dry concentrate	1304016-02	40	20130425
Euro OTC	Cholecalciferol dry concentrate	1502021-01	60	20150309
Euro OTC	Cholecalciferol dry concentrate	1602019	40	20160307*
Euro OTC	Cholecalciferol dry concentrate	1701053	40	20170208*
Euro OTC	Cholecalciferol dry concentrate	1707027	40	20171020*
Euro OTC	Cholecalciferol dry concentrate	1802014	40	20180223*
Euro OTC	Cholecalciferol dry concentrate	1801038	40	20180206*
Euro OTC	Cholecalciferol dry concentrate	1806003	40	20180618*
Euro OTC	Cholecalciferol dry concentrate	1812010	40	20190114*
Euro OTC	Cholecalciferol dry concentrate	1901050	40	20190221*
Euro OTC	Cholecalciferol dry concentrate	1906009	40	20190619*
Fagron	Cimetidine	2403109C03	40	20270320*
Fagron	Cimetidine	2403109C03	20	20270320*
Fagron	Cinchocaine hydrochloride	12F25-N10	40	1401148
Fagron	Cinchocaine hydrochloride	13G24-N05	40	20130826
Caelo	Cinchona bark, cut	11238512	40	1403463
Caelo	Cinchona bark, cut	13031007	40	20130207
Caelo	Cinchona bark, cut	14009304	40	AR-15-FG-007677-01
Caelo	Cinchona bark, cut	15301903	60	AR-17-FG-007831-01
Caelo	Cinnamon	12309902	40	pending
Caelo	Cinnamon	13304414	40	20130912
Caelo	Cinnamon	14175010	60	1505349
Caelo	Cinnamon	16114401	60	1704441
Caelo	Cinnamon rods (Ceylonese Cinnamon)	13241807	40	20130905

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Fagron	Cinnarizine	11L22-N13	40	20120104
Fagron	Cinnarizine	13H01-N07	40	1402306
Fagron	Cinnarizine	14D09-B01-294702	60	AR-16-FG-008930-01
Klenk	Cleavers goosegrass, cut	4731B110809	40	20110930
Caelo	Clove	12095805	40	pending
Caelo	Clove	16207804	60	1708676
Klenk	Clove	1260A150916	40	1708050
Caelo	Cocaine hydrochloride	16142710	40	1917T-01278
Caelo	Cocaine hydrochloride	18266104	40	1919M-01278
Caelo	Cocaine hydrochloride	17003902	40	1917S-01278
Caelo	Cocaine hydrochloride	16142710	40	1917T-01278
Caelo	Cocaine hydrochloride	18266104	40	1919M-01278
Fagron	Cocaine hydrochloride	14H27-B03-304551	40	1917R-01278
Fagron	Cocaine hydrochloride	18J01-B07-353630	40	1919I-01278
Fagron	Cocaine hydrochloride	16B11-B05-323386	40	1917Q-1278
Fagron	Cocaine hydrochloride	14H27-B03-304551	40	1917R-01278
Fagron	Cocaine hydrochloride	18J01-B07-353630	40	1919I-01278
Fagron	Codeine monohydrate	12C05-N05	40	0814I-01280
Fagron	Codeine monohydrate	12C05-N05	60	0814I-01280
Caelo	Codeine phosphate hemihydrate	16349702	40	2017C-01279
Caelo	Codeine phosphate hemihydrate	16169807	40	2017B-01279
Caelo	Codeine phosphate hemihydrate	18187906	40	1919M-01279
Caelo	Codeine phosphate hemihydrate	16349702	40	2017C-01279
Caelo	Codeine phosphate hemihydrate	16169807	40	2017B-01279
Caelo	Codeine phosphate hemihydrate	18187906	40	1919M-01279
Fagron	Codeine phosphate hemihydrate	16E17-B05-324109	40	2017A-01279
Th. Geyer	Codeine phosphate hemihydrate	067054	40	2017D-01279
Caelo	Colophony	15186804	60	AR-16-FG-005931-01
Caelo	Colophony	161332	40	20160510*
Caelo	Colophony	173014	40	20180102*
Caelo	Colophony	192081	40	20190731*
Caelo	Common wormwood herb	12016705	40	20120131
Euro OTC	Copper orotate dihydrate	1901040-01	50	20190319
Euro OTC	Copper orotate dihydrate	2203016	40	20220520*
Euro OTC	Copper orotate dihydrate	2203016	20	20220520*
Euro OTC	Copper(II) gluconate	2202011	40	20220301*
Euro OTC	Copper(II) gluconate	2202011	40	20220301*
Caelo	Copper(II) sulfate pentahydrate	162409	40	20160825*
Caelo	Coriander	12080904	40	pending
Caelo	Coriander	13299403	40	1412548
Caelo	Coriander	16010212	60	AR-17-FG-015965-01
EDQM	Cortisone acetate	6.0	20	CRS
Caelo	Cottonwood bud	12027505	40	20120131
Klenk	Cottonwood bud, pounded	3266B130826	40	1410178
Klenk	Cottonwood bud, pounded	3266B150624	60	20150701
Caelo	Couch grass rhizome, cut	12186702	40	20120629
Caelo	Cowberry leaf, cut	11334302	40	20111129
Caelo	Cumin	11378308	30	20120124
Euro OTC	Curcuma extract 95%	L1408013	60	20140815
Fagron	Curcumin	CP2403043	40	20240319*
Fagron	Curcumin	CP2404071	20	20240410*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Fagron	Curcumin	CP2403043	20	20240319*
Fagron	Curcumin	CP2403046	20	20240320*
Euro OTC	Cyclopentolate hydrochloride	2311002	40	20240322*
Euro OTC	Cyclopentolate hydrochloride	2409009	40	20241106*
Euro OTC	Cyclopentolate hydrochloride	2311002	20	20240322*
Euro OTC	Cyclopentolate hydrochloride	2409009	20	20241106*
Caelo	Daisy flower	11068306	40	20110323
Caelo	Damiana leaf, cut	11026608	40	20110221
Caelo	Dandelion herb without root	11217109	40	20110824
Caelo	Dandelion root	12363102	40	1403708
Caelo	Dandelion root	13329701	40	20131017
Caelo	Dandelion root	13329708	40	1411089
Klenk	Dandelion root	6621B151029	60	AR-17-FG-007535-01
Caelo	Dapsone	160735	60	20160405*
Caelo	Dapsone	16073502	40	20160405
Caelo	Dapsone	16073502	40	20160405
Caelo	Dapsone	170311	39	20170221*
Caelo	Dapsone	182792	40	20181214*
Caelo	Dapsone	191135	40	20190726*
Fagron	Deflazacort	6017-240501	40	20240518*
Fagron	Deflazacort	6017-240501	20	20240518*
Fagron	Deoxycholic acid	14A02-B32-303429	60	AR-16-FG-004648-01
Fagron	Deoxycholic acid	14A02-B32-303429	40	from supplier
Euro OTC	Devil's claw dry extract	2101020	40	20210203*
Euro OTC	Devil's claw dry extract	1210003-02	40	1707472
Euro OTC	Devil's claw dry extract	1210003-02	40	20151102
Euro OTC	Devil's claw dry extract	1210003-02	40	20151102
Caelo	Devil's claw root	12031806	40	20120222
Caelo	Devil's claw root	13298202	40	20130926
Sigma-Aldrich	Dexamethasone isonicotinate	Y0000538	40	CRS
Fagron	Dexamphetamine sulfate	16F09-B02-328352	40	2017A-03582
Fagron	Dexamphetamine sulfate	15H06-B04-313862	60	1316Q-03582
Fagron	Dexamphetamine sulfate	16D20-B01-321049	40	2017B-03582
Fagron	Dexamphetamine sulfate	16F09-B02-328352	40	2017A-03582
Caelo	Dihydrocodeine hydrogen tartrate	16106209	40	2017C-03065
Caelo	Dihydrocodeine hydrogen tartrate	15295910	40	2017B-03065
Caelo	Dihydrocodeine hydrogen tartrate	18115205	40	1919M-03065
Caelo	Dihydrocodeine hydrogen tartrate	16106209	40	2017C-03065
Caelo	Dihydrocodeine hydrogen tartrate	15295910	40	2017B-03065
Caelo	Dihydrocodeine hydrogen tartrate	18115205	40	1919M-03065
Fagron	Dihydrocodeine hydrogen tartrate	14K26-B04-306298	60	1516I-03065
Fagron	Dihydrocodeine hydrogen tartrate	15F18-B07-323388	40	2017A-03065
Th. Geyer	Dihydrocodeine hydrogen tartrate	067052	40	2017D-03065
Fagron	Dihydroergotamine mesilate	22A11-F01-384535	40	20220328
Fagron	Dihydroergotamine mesilate	22A11-F01-384535	20	20220328
Gatt-Koller	Dihydroergotamine mesilate	22J02560	40	20230109

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Gatt-Koller	Dihydroergotamine mesilate	22J02560	20	20230109
Caelo	Dill fruit	12289901	40	1403464
Caelo	Dill fruit	12342906	40	20121206
Caelo	Dill fruit	14018705	60	pending
Caelo	Dill fruit	23001474001	30	20231010
Klenk	Dill fruit	2680A170222	60	20170308
Caelo	Dill herb, cut	11295107	40	pending
Caelo	Dill herb, cut	13007602	40	1402204
Caelo	Dill herb, cut	13007610	40	20130208
Fagron	Dimenhydrinate	21J13-B12-223576	40	20220117*
Fagron	Dimenhydrinate	21J13-B12-223576	20	20220117*
abcr GmbH	Dimercaptosuccinic acid	1005874	39	from supplier
Safic-Alcan	Dimercaptosuccinic acid	20180130	40	from supplier
Caelo	Dimethyl fumarate	13269801	60	1506634
Euro OTC	Dimethyl fumarate	1410013-01	60	20141125
Euro OTC	Dimethyl fumarate	1601013-01	40	20160204
Fagron	Diosmin	DSM240603	40	20241031*
Fagron	Diosmin	DSM240602	20	20241031*
Fagron	Diosmin	DSM240401	20	20241031*
Fagron	Diosmin	DSM240603	20	20241031*
Sigma-Aldrich	Disodium hydrogen phosphate	102544017	40	not required
Fagron	Doxazosin mesylate	DM0060624	40	20240705*
Fagron	Doxazosin mesylate	DM0060624	20	20240705*
Fagron	Drofenine hydrochloride	13I09-N05	40	20130524
Fagron	Drofenine hydrochloride	15G01-B04-323028	40	20150709
Fagron	Drofenine hydrochloride	15G01-B04-330979	40	AR-17-FG-015434-02
Fagron	Drofenine hydrochloride	15G01-B04-330979	40	20150709
Fagron	Drofenine hydrochloride	18A18-B99-345993	40	20180308
EDQM	Econazole	1.0	10	CRS
Caelo	Elder berries	12267807	40	1403466
Caelo	Elder berries	13367704	40	1410179
Klenk	Elder berries	3010A120202	40	pending
Caelo	Elder flower	12221902	40	20120821
Klenk	Elder leaf, cut	2321B130221	60	20130226
Caelo	Elecampane rhizome, cut	12113303	40	20120427
Klenk	Elecampane rhizome, cut	6341B120611	40	20120620
Caelo	Eleutherococcus, cut	10381814	30	20110113
Caelo	Elm bark, cut	10347205	60	20101223
Yino Pharma	Enoxaparin sodium	YN010232210003	40	20230524*
Yino Pharma	Enoxaparin sodium	YN010232210003	20	20230524*
Caelo	Equisetum stem	10375515	40	20110114
Fagron	Ergotamine tartrate	13H02-N01	100	20120412
Fagron	Ergotamine tartrate	13I24-B10-288648	50	20131024
Fagron	Ergotamine tartrate	13I24-B10-288650	60	20131024
Fagron	Ergotamine tartrate	15B16-B05-308418	45	9384
Fagron	Ergotamine tartrate	15B16-B05-308417	40	20150302
Fagron	Ergotamine tartrate	15B16-B05-308418	45	9384
Fagron	Ergotamine tartrate	15B16-B05-308417	40	20150302
EDQM	Erythromycin estolate	1.4	40	CRS
Fagron	Erythromycin estolate	EV/EE-085/24	40	20240803*
Fagron	Erythromycin estolate	EV/EE-085/24	20	20240803*
EDQM	Erythromycin stearate	1.2	40	CRS
Fagron	Ethyl hydrogen fumarate	14C12-B07-292760	60	1410436
Fagron	Ethyl hydrogen fumarate	14C12-B07-292760	60	20140417
Euro OTC	Ethyl hydrogen fumarate calcium	1310029-01	60	20131126
Euro OTC	Ethyl hydrogen fumarate calcium	1306012-01	60	1505456

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Euro OTC	Ethyl hydrogen fumarate calcium	1510005	60	20151030*
Euro OTC	Ethyl hydrogen fumarate calcium	1601011	60	20160114*
Euro OTC	Ethyl hydrogen fumarate calcium	2001042	40	20200331*
Fagron	Ethyl hydrogen fumarate calcium	13B25-N08	60	1411090
Euro OTC	Ethyl hydrogen fumarate magnesium	1306014-01	60	20130805
Euro OTC	Ethyl hydrogen fumarate magnesium	1510006	60	20151030*
Euro OTC	Ethyl hydrogen fumarate magnesium	1601010	60	20160114*
Euro OTC	Ethyl hydrogen fumarate magnesium	1510006-01	40	AR-18-FG-000547-01
Fagron	Ethyl hydrogen fumarate magnesium	13G10-N01	60	1411091
Klenk	Euphrasy herb	3871B100713	40	20100721
Bombastus	Fennel, bitter	289870	60	AR-15-FG-008161-01
Bombastus	Fennel, bitter	24000576	30	20240129
Caelo	Fennel, bitter	12094708	40	pending
Caelo	Fennel, bitter	12167102	40	20120705
Caelo	Fennel, bitter	13413702	40	1412549
Caelo	Fennel, bitter	14376403	60	20150108
Caelo	Fennel, bitter	161603	60	20160718*
Caelo	Fennel, bitter	17020610	40	1708048
Caelo	Fennel, bitter	23002233002	30	20231212
Klenk	Fennel, bitter	2880N120418	40	1412547
Klenk	Fennel, bitter	2880N120418	40	AR-15-FG-002805-02
Klenk	Fennel, bitter	2860A140613	60	AR-15-FG-008160-01
Klenk	Fennel, sweet	2870A110412	40	pending
Klenk	Fennel, sweet	2870A130304	40	1405154
Fagron	Fentanyl citrate	16E26-B01-525360	40	2017A-03686
Fagron	Fentanyl citrate	16E26-B01-525360	40	2017A-03686
Caelo	Fenugreek	11313204	40	20111122
Caelo	Fenugreek, powdered	12149605	40	20120629
Caelo	Fenugreek, powdered	15308704	60	AR-17-FG-006625-01
Klenk	Fenugreek, powdered	7264B130205	40	1408080
Klenk	Fenugreek, powdered	7264A151001	60	AR-16-FG-014493-01
Euro OTC	Fexofenadine hydrochloride	2310018	20	20240222*
Caelo	Flax weed herb	13007505	40	1403462
Caelo	Flax weed herb	14005309	60	20140203
Caelo	Flax weed herb	20003289005	30	20201130
Audor	Fluconazole	AP061502911F	60	AR-16-FG-008733-01
Audor	Fluconazole	AP061502911F	40	AR-16-FG-014225-01
Audor	Fluconazole	AP061502911F	40	20150821
Audor	Fluconazole	APAFLNC0217023F	40	20170421
Audor	Fluconazole	AP061502911F	60	20150821
Audor	Fluconazole	AP061502911F	40	20150821
Audor	Fluconazole	AP061502911F	40	20150821
Caelo	Frangula bark	12185901	40	20120710
Caelo	Frankincense	12120005	40	1402495
Caelo	Frankincense	13112801	40	20130503
Euro OTC	Frankincense extract 80%	1308020-01	60	8958
Euro OTC	Frankincense extract 80%	1602008	60	20160215*
Euro OTC	Frankincense extract 80%	1602008	60	20160215*
Euro OTC	Frankincense extract 80%	1611023-01	60	9889
Caelo	Fraxinella root, cut	10189103	40	20100804
Caelo	Fraxinella root, cut	11314705	40	pending

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Fraxinella root, cut	11314705	80	20111115
Caelo	Fraxinella root, cut	14110802	60	20140428
Caelo	Fumitory	12103402	40	20120425
Caelo	Galangal root	12125001	40	20120516
Caelo	Galangal root	11375904	40	20120109
Caelo	Galangal root	12330305	40	1403491
Caelo	Galangal root	11375909	40	1403324
Caelo	Galangal root	12330308	40	20121203
Caelo	Galangal root	14159504	60	1511617
Klenk	Galeopsis herb, cut	3911A090219	40	20120426
Fagron	gamma-Aminobutyric acid	1524040601	40	20240406*
Fagron	gamma-Aminobutyric acid	1524040601	20	20240406*
Caelo	Garden violet, cut	10292002	40	pending
Caelo	Garden violet, cut	13038703	40	1403481
Caelo	Garden violet, cut	13232103	40	20130821
Caelo	Gentian root	12244603	40	20120914
Caelo	Gentian root, powdered	12007103	50	1403630
Caelo	Gentian root, powdered	12007106	40	20120117
Caelo	Gentian root, powdered	13410503	40	1508394
Caelo	Ginger	14120701	40	20140516
Caelo	Ginger	13321904	40	20131016
Klenk	Ginger, peeled, powdered	6954B140724	60	AR-15-FG-014915-01
Klenk	Ginger, peeled, powdered	6954B150325	60	1606616
Klenk	Ginger, peeled, powdered	6954B170127	60	1708675
Fagron	Ginkgo biloba dry extract (NLT 24% of total flavonoids)	24H27-B082	40	20240925*
Fagron	Ginkgo biloba dry extract (NLT 24% of total flavonoids)	24H27-B082	20	20240925*
Caelo	Ginkgo extract	12192505	40	1403672
Caelo	Ginkgo leaf	12151703	40	20120613
Caelo	Ginkgo leaf	13340904	40	1411088
Caelo	Ginkgo leaf	13340907	60	20131028
Caelo	Ginkgo leaf	16281501	60	1708047
Caelo	Ginkgo leaf	24100105001	30	20241011
Klenk	Ginkgo leaf	2461B220718-01	30	20220802
Caelo	Ginseng root	12080208	40	20120329
Caelo	Ginseng root	11349206	40	20111227
Caelo	Ginseng root	13341008	40	20131029
Caelo	Ginseng root	13237805	40	20130816
Fagron	Glucosamine sulfate potassium chloride	TSM-K-2404003	40	20240928*
Fagron	Glucosamine sulfate potassium chloride	TSM-K-2404002	20	20240928*
Fagron	Glucosamine sulfate potassium chloride	TSM-K-2404003	20	20240928*
Fagron	Glucosamine sulfate potassium chloride	TSM-K-2404001	20	20240928*
abcr GmbH	Glycyrrhizic acid	1222024	40	from supplier
Klenk	Goat's rue, cut	3901C110905	40	20111005
Klenk	Greater celandine herb	3731K120904	40	20120920
Klenk	Greek mountain herb, cut	4511K130314	40	20130402
Klenk	Green tea	5100A100611	40	20120126
Euro OTC	Griffonia seed extract	1810009	40	20181025*
Fagron	Griffonia seed extract (L-5 Hydroxytryptophan)	20240412	40	not required
Fagron	Griffonia seed extract (L-5 Hydroxytryptophan)	2024020	40	not required

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Fagron	Griffonia seed extract (L-5 Hydroxytryptophan)	20240414	40	not required
Fagron	Griffonia seed extract (L-5 Hydroxytryptophan)	20240412	20	not required
Fagron	Griffonia seed extract (L-5 Hydroxytryptophan)	2024020	40	not required
Fagron	Griffonia seed extract (L-5 Hydroxytryptophan)	20240414	20	not required
Caelo	Guaiacum wood	11352001	40	1406340
Caelo	Guaiacum wood	11352012	40	20111222
Caelo	Guaiacum wood	13343802	40	20131113
Caelo	Hamamelis bark, cut	12361301	40	20121213
Caelo	Hamamelis bark, cut	12361303	40	20121213
Caelo	Hamamelis leaf	10102915	40	20100517
Caelo	Hamamelis leaf	13269902	40	1405176
Caelo	Hamamelis leaf	13269904	40	20130924
Caelo	Hawthorn flower	10157201	40	20100701
Caelo	Hawthorn flower	13010403	40	20130130
Caelo	Hawthorn fruit	11183010	40	20110701
Caelo	Hawthorn fruit	11278205	30	20111025
Caelo	Hawthorn leaf with flower	10273515	40	20101028
Caelo	Hawthorn leaf with flower	10273513	40	20101028
Caelo	Hawthorn leaf with flower	13276706	40	20130927
Galke	Hawthorn leaf with flower	21126	40	20121109
Caelo	Heather flower, rubbed	10270508	40	20101018
Caelo	Heather, cut	11011209	40	20110218
Caelo	Henna powder	12122302	40	from supplier
Caelo	Henna powder	12267304	40	from supplier
Caelo	Hop strobile	12008305	40	20120213
Caelo	Hop strobile	12221802	40	20120817
Caelo	Hop strobile	23001009005	30	20230823
Caelo	Horse chestnut leaf	11063503	40	20110315
Fagron	Hydrocortisone butyrate	13I26-N01	60	AR-15-FG-000944-01
Fagron	Hydrocortisone butyrate	14D23-B01-296716	60	20140509
Fagron	Hydrocortisone butyrate	13I26-N01	60	20130920
Fagron	Hydrocortisone butyrate	16F20-B05-323903	40	20160805
Fagron	Hydrocortisone butyrate	15J12-B03-322394	40	20151028
Fagron	Hydrocortisone butyrate	16J21-B01-333229	40	20161206
Fagron	Hydrocortisone butyrate	16J21-B01-333229	40	20161206
Fagron	Hydrocortisone butyrate	14D23-B01-296716	48	20140509
Fagron	Hydrocortisone butyrate	13I26-N01	45	20130920
Fagron	Hydrocortisone butyrate	16F20-B05-323903	20	20160805
Fagron	Hydrocortisone butyrate	15J12-B03-322394	25	20151028
Fagron	Hydrocortisone butyrate	15J12-B03-322394	22	20151028
Fagron	Hydrocortisone butyrate	16J21-B01-333229	37	20161206
Fagron	Hydrocortisone butyrate	16J21-B01-333229	36	20161206
EDQM	Hydrocortisone hydrogen succinate	3.0	40	CRS
Caelo	Hydromorphone hydrochloride	16123804	40	1917R-01334
Caelo	Hydromorphone hydrochloride	18316002	40	1919M-01334
Caelo	Hydromorphone hydrochloride	16123804	40	1917R-01334
Caelo	Hydromorphone hydrochloride	18316002	40	1919M-01334
Fagron	Hydromorphone hydrochloride	17F01-B01-337510	40	1919I-01334
Fagron	Hydromorphone hydrochloride	15L08-B08-316877	40	1917Q-01334

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Fagron	Hydromorphone hydrochloride	17F01-B01-337510	40	1919I-01334
Caelo	Hydroxychloroquine sulfate	20001292	40	20200427*
Fagron	Hydroxytryptophan (L-5-)	21G12-B06-213943	40	20211103
Fagron	Hydroxytryptophan (L-5-)	23G12-B14-231034	40	20230817
Fagron	Hydroxytryptophan (L-5-)	21G12-B06-213943	11	20211103
Fagron	Hydroxytryptophan (L-5-)	23G12-B14-231034	20	20230817
Fagron	Indigo carmine	13K12-N01	40	1601099
Spinnrad	Inulin	1112300433	40	from supplier
Caelo	Iodine	181635	40	20180704*
Caelo	Iron(II) sulfate heptahydrate	11340509	40	1401568
Caelo	Iron(III) chlorid hexahydrate	12354703	40	1401391
Caelo	Iron(III) chlorid hexahydrate	22000819	40	20220323*
Caelo	Iron(III) chlorid hexahydrate	24002426	40	20241021*
Caelo	Iron(III) chlorid hexahydrate	22000819	10	20220323*
Caelo	Iron(III) chlorid hexahydrate	24002426	20	20241021*
Caelo	Iron(III) sulfate hydrate	170991	40	20170523*
EDQM	Isoconazole	1.1	40	CRS
EDQM	Isoconazole nitrate	1.1	40	CRS
Caelo	Isomalt	170812	40	20170421*
Caelo	Ispaghula husks	12148103	40	20120628
Caelo	Ispaghula seed	11185807	40	20110727
Caelo	Ivy leaf, cut	11229505	40	20110829
Caelo	Ivy leaf, cut	13276304	40	20130913
Caelo	Jasmine flower	12143201	40	20120606
Caelo	Java tea	12225702	40	20120809
Caelo	Java tea	13258805	40	20130826
Klenk	Java tea	2221B110718	40	20120605
Caelo	Juniper berry	12028609	40	20120207
Caelo	Juniper berry	13267210	40	20130828
Caelo	Juniper berry, pounded	12278903	40	1405296
Klenk	Juniper berry, powdered	2894B130320	40	1411362
Klenk	Juniper berry, powdered	2894B150922	60	1704439
Euro OTC	Kaolin, heavy	2303011	40	20230412*
Euro OTC	Kaolin, heavy	2303011	20	20230412*
Caelo	Kaolin, red	12093503	40	from supplier
Caelo	Kap-Aloe	14087106	60	20140404
Inresa	Ketoprofen	F1300183	60	AR-15-FG-009572-01
Inresa	Ketoprofen	F1300182	60	20150617
Euro OTC	Ketotifen hydrogen fumarate	2109027	50	20211026*
Euro OTC	Ketotifen hydrogen fumarate	2304008	40	20230420*
Euro OTC	Ketotifen hydrogen fumarate	2109027	10	20211026*
Euro OTC	Ketotifen hydrogen fumarate	2304008	20	20230420*
Caelo	Kidney vetch, coarsely rubbed	10249206	40	20100928
Caelo	Knotgrass	14079304	40	20140402
Klenk	Knotgrass	4301A120912	40	20120924
Caelo	Lady's bedstraw herb	11265103	40	20111006
Klenk	Lady's bedstraw herb	3921B101012	40	20111216
Caelo	Lapacho wood, cut	12239305	40	20120831

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Lapis Pumicis	180533	40	20180222*
Caelo	Laurel leaf	12299103	40	20121108
Klenk	Laurel leaf, powdered	2124A110329	40	1411032
Klenk	Laurel leaf, powdered	2124A110329	60	20140310
Bombastus	Lavender flower	24000229	30	20240111
Caelo	Lavender flower	12088003	60	20120411
Caelo	Lavender flower	13336005	40	from supplier
Caelo	Lavender flower	23001761001	30	20231129
Euro OTC	L-Carnitine tartrate	1708023	40	20170907*
Euro OTC	L-Carnitine tartrate	2007043	40	20200810*
Euro OTC	L-Carnitine tartrate	2105018	50	20210625*
Euro OTC	L-Carnitine tartrate	2207004	40	20221213*
Euro OTC	L-Carnitine tartrate	2305008	40	20230718*
Fagron	L-Carnitine tartrate	10100220240309	20	20260228*
Pharmorgana	L-Carnitine tartrate	1000160672	40	from supplier
Pharmorgana	L-Carnitine tartrate	1000170113	40	from supplier
Caelo	Lemon peel, cut	12217402	40	20120823
Caelo	Lemon verbena leaf, cut	12137505	40	20120605
Caelo	Lemon verbena leaf, cut	12137503	40	20120605
Flora Apot…	Levamisole hydrochloride	LV19305	40	from supplier
Caelo	Lime flower	11086305	55	20110420
Caelo	Linseed	12092102	60	20120402
Caelo	Linseed	13296703	40	20131008
Caelo	Liqourice root	12267103	40	20120917
Caelo	Liqourice root, peeled	12227101	40	20120813
Caelo	Liqourice root, peeled	12227106	40	20120813
Caelo	Liquorice	13068904	40	20130315
Caelo	Liquorice	14050601	60	from supplier
Caelo	Liquorice	13180904	60	pending
Fagron	L-Malic acid	15J09-B03-313987	60	9346
Fagron	L-Malic acid	15J09-B03-313987	40	20151106
Fagron	L-Malic acid	15J09-B03-313987	40	20151106
Fagron	L-Malic acid	16J06-B98-327269	40	20161117
Fagron	L-Malic acid	16J06-B98-327269	40	20161117
Fagron	L-Malic acid	17E23-B03-335458	40	20170621
Caelo	Locust bean gum, powdered	10376516	40	20110106
Caelo	Locust bean gum, powdered	13379403	40	from supplier
Fagron	Losartan potassium	D5440-24-006	20	20240410*
Caelo	Lovage root	11181609	40	20110629
Fagron	Macrogols 6000 powder	14C11-B01-296014	60	20140324
Fagron	Macrogols 6000 powder	14J17-B01-309247	60	20141027
Fagron	Macrogols 6000 powder	14J17-B01-309247	60	AR-16-FG-011486-01
Caelo	Magensium hydrogen phosphate trihydrate	12181911	40	20120716
Fagron	Magnesium aspartate dihydrate	15I24-B89-313231	60	AR-16-FG-008660-03
Fagron	Magnesium aspartate dihydrate	15I24-B89-313231	60	20151016
Fagron	Magnesium aspartate dihydrate	17C21-B05-333111	40	20170412
Fagron	Magnesium aspartate dihydrate	18D23-B01-350069	40	20180625
Euro OTC	Magnesium carbonate, light, basic	1711011-01	40	20171116
Euro OTC	Magnesium carbonate, light, basic	2201023	40	20220317*
Euro OTC	Magnesium carbonate, light, basic	2201023	20	20220317*
VWR Intern…	Magnesium chloride 4,5-hydrate	22E054108	40	not required

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Magnesium hydroxide	16253301	30	20160921
Euro OTC	Magnesium oxide, heavy	1709011-02	40	20170915
Caelo	Magnesium oxide, light	180818	40	20180322*
Caelo	Magnesium sulfate, dried	172990	40	20171129*
Euro OTC	Magnesium trisilicate	1608024-01	40	20160908
Bombastus	Maize style	274920	40	66662
Caelo	Maize style	10325906	40	20101217
Caelo	Maize style	13381501	40	20140103
Klenk	Maize style	5581A111206	40	20111214
Caelo	Male speedwell wort	12162503	40	20120703
Caelo	Mallow flower	12187405	40	20120719
Caelo	Mallow leaf	12153403	40	20120614
Caelo	Manna	11308907	60	20111117
Caelo	Manna	13127007	40	20130424
Caelo	Manna, powdered	11308807	40	1403534
Caelo	Manna, powdered	14001401	40	20140115
Caelo	Marian thistle fruit	11126703	40	20110608
Caelo	Marian thistle fruit	13342002	40	from supplier
Caelo	Marian thistle herb	10365601	40	20110111
Caelo	Marshmallow leaf	12328206	40	20121114
Caelo	Masterwort root, cut	12101804	60	20120405
Caelo	Masterwort root, cut	13341204	40	20131030
Caelo	Maté leaf	11091707	40	20110428
Caelo	Maté leaf	13118004	40	20130506
Caelo	Maté leaf	24100015001	30	20240610
Galke	Maté leaf	21684	40	from supplier
Bombastus	Matricaria flower	24004030	30	20240926
Caelo	Matricaria flower	12294804	40	20121113
Caelo	Matricaria flower	24100110001	30	20241031
Caelo	Matricaria flower for bathing	12115805	40	from supplier
Klenk	Meadowsweet	4541A120313	60	20120327
Caelo	Meadowsweet flower, rubbed	12275701	40	20121023
EDQM	Medroxyprogesterone - acetate	3.0	40	CRS
Bombastus	Mellisa leaf	24001976	30	20240423
Caelo	Mellisa leaf	12032318	40	20120302
Caelo	Mellisa leaf	24100001001	30	20240502
Galke	Mellisa leaf	22218	40	from supplier
Klenk	Mellisa leaf	2161A090630	130	20120328
Klenk	Mellisa leaf	2161A121029	55	20121113
Fagron	Metformin hydrochloride	22C04-B02-219168	40	20220625
Fagron	Metformin hydrochloride	23H03-B10-234791	40	20230925
Fagron	Metformin hydrochloride	24B27-B04-239307	40	250201361
Fagron	Metformin hydrochloride	22C04-B02-219168	20	20220625
Fagron	Metformin hydrochloride	23H03-B10-234791	20	20230925
Fagron	Metformin hydrochloride	24B27-B04-239307	20	250201361
Caelo	Methadone hydrochloride	16135309	40	1917R-02949
Caelo	Methadone hydrochloride	18132413	40	1919Q-02949
Caelo	Methadone hydrochloride	16135309	40	1917R-02949
Caelo	Methadone hydrochloride	18132413	40	1919Q-02949
Fagron	Methadone hydrochloride	18G02-B02-355990	40	1919I-02949
Fagron	Methadone hydrochloride	16F24-B02-323183	40	1917Q-02949
Fagron	Methadone hydrochloride	18G02-B02-355990	40	1919I-02949
Th. Geyer	Methadone hydrochloride	067055	40	1917S-02949
Th. Geyer	Methadone hydrochloride	067055	40	1917S-02949
EDQM	Methylprednisolone acetate	2.0	20	CRS
EDQM	Methylprednisolone hydrogen succinate	3.0	40	CRS

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Methylrosanilinium chloride	12276308	40	1509299
Fagron	Methylrosanilinium chloride	13H28-N03	60	20130625
Fagron	Methylrosanilinium chloride	13H28-N03	60	AR-15-FG-004742-01
USP	Metoprolol succinate	R11100	40	CRS
Fagron	Metronidazole benzoate	22A17-B10-216356	40	20220607
Fagron	Metronidazole benzoate	22A17-B10-216356	20	20220607
Th. Geyer	Mg-Ca-K colamine phosphate	54610	40	from supplier
Th. Geyer	Mg-Ca-K colamine phosphate	54610	40	from supplier
Dr. K. Hol...	Miconazole	029C064	40	20190415
Fagron	Midazolam	13K05-N01	40	0914E-07393
Fagron	Midazolam	14C12-B31-313222	60	1516A-07393
Fagron	Midazolam	16J03-B09-326963	40	1917Q-07393
Fagron	Midazolam	17J16-B01-342518	40	1919I-07393
Fagron	Midazolam	13K05-N01	60	0914E-07393
Fagron	Midazolam	14C12-B31-313222	60	1516A-07393
Fagron	Midazolam	16J03-B09-326963	30	1917Q-07393
Fagron	Midazolam	17J16-B01-342518	40	1919I-07393
Caelo	Midazolam hydrochloride	15224611	40	1917S-03538
Caelo	Midazolam hydrochloride	15224611	30	1917S-03538
Fagron	Midazolam hydrochloride	15J07-B01-320717	40	1917Q-03538
Fagron	Midazolam hydrochloride	18B28-B05-354856	40	1919J-03538
Fagron	Midazolam hydrochloride	15J07-B01-320717	30	1917Q-03538
Fagron	Midazolam hydrochloride	15H04-B03-314396	30	1917R-03538
Fagron	Midazolam hydrochloride	18B28-B05-354856	40	1919J-03538
Fagron	Minoxidil sulfate	01801022406016	40	20241230*
Fagron	Minoxidil sulfate	01801022407017	20	20241230*
Fagron	Minoxidil sulfate	01801022406016	20	20241230*
Fagron	Minoxidil sulfate	01801022405015	20	20240930*
MEDICHEM S.A.	Mirtazapine	A-180132	50	20180312
MEDICHEM S.A.	Mirtazapine	A-210100	50	20210211
MEDICHEM S.A.	Mirtazapine	2024A152	40	20241023
MEDICHEM S.A.	Mirtazapine	A-180132	50	20180312
MEDICHEM S.A.	Mirtazapine	A-210100	50	20210211
MEDICHEM S.A.	Mirtazapine	2024A152	40	20241023
Caelo	Morphine hydrochloride	15439411	40	1917R-01879
Caelo	Morphine hydrochloride	18188607	40	1919Q-01879
Caelo	Morphine hydrochloride	16184605	40	1917S-01879
Caelo	Morphine hydrochloride	15439411	40	1917R-01879
Caelo	Morphine hydrochloride	18188607	40	1919Q-01879
Fagron	Morphine hydrochloride	16D21-B02-322088	40	1917Q-01879
Fagron	Morphine hydrochloride	17F22-B01-338170	40	1919I-01879
Fagron	Morphine hydrochloride	16D21-B02-322088	40	1917Q-01879
Fagron	Morphine hydrochloride	17F22-B01-338170	40	1919I-01879
Caelo	Morphine sulfate	12153212	40	0914F-07776
Caelo	Morphine sulfate	11333103	40	0914E-07776
Caelo	Morphine sulfate	15255703	60	1416Q-07776
Caelo	Morphine sulfate	15295802	40	1917R-07776
Caelo	Morphine sulfate	17331510	40	2319I-07776
Caelo	Morphine sulfate	12153212	60	0914F-07776
Caelo	Morphine sulfate	11333103	60	0914E-07776
Caelo	Morphine sulfate	15255703	60	1416Q-07776
Caelo	Morphine sulfate	15295802	40	1917R-07776
Caelo	Morphine sulfate	17331510	40	2319I-07776
Fagron	Morphine sulfate	13J07-N04	40	0914G-07776
Fagron	Morphine sulfate	14F02-B06-315405	40	1917Q-07776
Fagron	Morphine sulfate	13J07-N04	60	0914G-07776
Fagron	Morphine sulfate	14F02-B06-315405	40	1917Q-07776
Klenk	Motherwort	4071A121211	40	20130104

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Mullein flower	11366403	40	20120105
Caelo	Mullein flower, cut	11233402	60	20110914
Caelo	Myrrh	12269901	40	1403470
Klenk	Myrrh	3355B120628	40	AR-15-FG-000945-01
Euro OTC	N-Acetyltyrosine	2307037	40	20230915*
Euro OTC	N-Acetyltyrosine	2307037	20	20230915*
Caelo	Nettle leaf	12184702	40	20120628
Galke	Nettle leaf	21238	40	from supplier
Caelo	Nettle root	11254903	40	20111121
Caelo	Nettle seed	12131507	40	1402203
Caelo	Nettle seed	11126211	40	pending
Caelo	Nettle seed	13387110	40	1410300
Klenk	Nettle seed	7470A111117	40	pending
Klenk	Nettle seed	7470A221024-02	30	20221122
Caelo	Nutmeg	12067304	40	20120320
Caelo	Nutmeg	13266002	40	20130906
Caelo	Nutmeg	22002543003	30	20221004
Klenk	Nutmeg	7320A121002	40	20121012
Caelo	Oak bark	10348617	40	20101221
Caelo	Oak bark	11351207	40	1403492
Caelo	Oak bark	13360306	40	20131203
Caelo	Oak bark, powdered	11235004	40	20110909
Caelo	Oat straw	11280008	40	20111020
Caelo	Olive leaf	11270106	40	20111013
Caelo	Olive leaf	12316808	60	AR-15-FG-001051-01
Fagron	Ondansetron hydrochloride dihydrate	24H07-H03-00987	40	20240808
Fagron	Ondansetron hydrochloride dihydrate	24H07-H03-00987	20	20240808
Fagron	Orlistat	2406002	40	20240906*
Fagron	Orlistat	6012307007-01	40	20230524*
Fagron	Orlistat	6012307004-01	20	20240523*
Fagron	Orlistat	6012307003-02	20	20240526*
Fagron	Orlistat	2406002	20	20240906*
Fagron	Orlistat	6012307007-01	20	20230524*
Caelo	Orris root	12206802	40	20120813
Caelo	Oxycodone hydrochloride	12268908	40	0914E-07734
Caelo	Oxycodone hydrochloride	12034515	40	0914F-07734
Caelo	Oxycodone hydrochloride	12268914	60	1416Q-07734
Caelo	Oxycodone hydrochloride	12268913	60	1416R-07734
Caelo	Oxycodone hydrochloride	15220205	40	2017A-07734
Caelo	Oxycodone hydrochloride	17270202	40	1919Q-07734
Caelo	Oxycodone hydrochloride	12268908	60	0914E-07734
Caelo	Oxycodone hydrochloride	12034515	60	0914F-07734
Caelo	Oxycodone hydrochloride	12268914	60	1416Q-07734
Caelo	Oxycodone hydrochloride	12268913	60	1416R-07734
Caelo	Oxycodone hydrochloride	15220205	40	2017A-07734
Caelo	Oxycodone hydrochloride	17270202	40	1919Q-07734
EDQM	Oxytetracycline	8.0	40	CRS
Caelo	Pale coneflower root	12244501	40	20120817
Caelo	Pale coneflower root	14120602	40	20140417
Klenk	Parsley herb, rubbed	4262A091116	60	20110719
Caelo	Parsley root	12080301	40	20120329
Klenk	Passionflower herb	4231A120329	40	20120419
Klenk	Peony root, cut	6421B120327	60	20120403
Caelo	Pepper	12192311	40	1403490
Caelo	Pepper	13221114	40	20130805
Caelo	Pepper	23001971003	30	-
Caelo	Pepper	24100075001	30	20240924
Bombastus	Peppermint leaf	24003080	30	20240716

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Peppermint leaf	11294401	40	20111104
Caelo	Peppermint leaf	12321503	130	20121026
Caelo	Peppermint leaf	13288303	40	20131002
Caelo	Peppermint leaf	24100035002	30	20240717
Galke	Peppermint leaf	20244	40	20120518
Galke	Peppermint leaf	19537	40	from supplier
Fagron	Phenibut	24H26-B009	40	20240917*
Fagron	Phenibut	24H26-B009	20	20240917*
Fagron	Phenobarbital	16G20-B04-328344	40	2017B-01040
Fagron	Phenobarbital	16G20-B04-328344	40	2017B-01040
Th. Geyer	Phenobarbital	067056	40	2017A-01040
Caelo	Phenol	23002846	40	20231108*
Caelo	Phenol	24001307	40	20240701*
Caelo	Phenol	24001307	20	20240701*
Fagron	Phenolphthalein	20G24-F01-375331	40	20201202
Fagron	Phenolphthalein	22J07-B02-227243	40	20221102
Fagron	Phenolphthalein	20G24-F01-375331	20	20201202
Fagron	Phenolphthalein	22J07-B02-227243	20	20221102
Caelo	Pine sprouts, cut	11164708	60	20110610
Caelo	Pine sprouts, cut	13256105	40	20130828
Caelo	Piper cubeba	11081903	40	20110404
Fagron	Piroxicam	VLSPRM0022425	40	20240512*
Fagron	Piroxicam	VLSPRM0022425	20	20240512*
Caelo	Podophyllum resin (from podophyllum peltatum)	12287810	40	1405242
Caelo	Potassium bromide	11208211	40	20110803
Caelo	Potassium carbonate	180995	40	20180412*
Caelo	Potassium hydroxide	180083	40	20180118*
Caelo	Potassium iodide	11090222	40	20110415
Caelo	Potassium metabisulfite	12325906	40	20121106
Caelo	Potassium monohydrogen phosphate	12366501	40	10401307
Caelo	Potassium monohydrogen phosphate	21001529	50	20210712*
Caelo	Potassium nitrate	12236703	40	20120807
Euro OTC	Potassium orotate	1203038V-02	40	from supplier
Flora Apot…	Potassium orotate	ORK00119	40	from supplier
Euro OTC	Potassium permanganate	1708016-02	40	20170824
Caelo	Potassium sodium tartrate tetrahydrate	12030207	40	20120213
Caelo	Potassium sodium tartrate tetrahydrate	13216605	40	1404530
Caelo	Potassium sodium tartrate tetrahydrate	14376001	60	20150204
Caelo	Potassium sodium tartrate tetrahydrate	15375607	40	20151030
Caelo	Potassium sodium tartrate tetrahydrate	172577	40	20171128*
Caelo	Potassium sodium tartrate tetrahydrate	20000750003	40	20200506
Caelo	Potassium tartrate hemihydrate	13331101	40	1403536
Caelo	Potassium tartrate hemihydrate	13331104	60	20131002
Caelo	Potassium tartrate hemihydrate	15167701	60	20150608
Caelo	Potassium tartrate hemihydrate	160289	60	20160405*
Caelo	Potassium tartrate hemihydrate	182203	40	20180907*

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Potassium tartrate hemihydrate	192911	40	20191125*
Caelo	Potassium tartrate hemihydrate	193079	40	20191125*
Sigma-Aldrich	Prednisolone pivalate	P2805000	40	CRS
Caelo	Primrose flower	11206806	100	20110809
Caelo	Primrose flower	11268002	40	20111007
Caelo	Primrose root, cut	12064506	40	20120319
Caelo	Promethazine hydrochloride	13119214	60	20130506
Caelo	Promethazine hydrochloride	161466	40	20160621*
Caelo	Promethazine hydrochloride	17058601	40	20170310
Caelo	Promethazine hydrochloride	170586	40	20170310*
Caelo	Propolis extract (96%) 2:1	11124120	40	1403460
Caelo	Propolis extract (96%) 2:1	13396103	40	20131212
Caelo	Propolis extract (96%) 2:1	13396103	40	20131212
Caelo	Psyllium seed	10291206	40	pending
Caelo	Psyllium seed	10291205	80	20101119
Caelo	Psyllium seed	13305903	40	pending
Fagron	Pullulan	24H27-B078	20	20240916*
Caelo	Pumpkin seed	12249002	40	1404542
Caelo	Pumpkin seed	12249006	40	20120917
Caelo	Quinine dihydrochloride	16269603	40	1709386
Caelo	Quinine dihydrochloride	16269603	40	20161021
Caelo	Quinine dihydrochloride	162696	40	20161021*
Caelo	Quinine dihydrochloride	172129	40	20173008*
Caelo	Quinine dihydrochloride	172072	40	20170830*
Caelo	Quinolinol sulfate potassium sulfate	13071104	40	1403095
Caelo	Quinolinol sulfate potassium sulfate	13403501	60	20131218
Caelo	Quinolinol sulfate potassium sulfate	15147704	40	20150618
Caelo	Quinolinol sulfate potassium sulfate	15147704	40	20150618
Caelo	Quinolinol sulfate potassium sulfate	162218	40	20160808*
Caelo	Quinolinol sulfate potassium sulfate	16221809	40	20160808
Caelo	Ramsons herb	12380801	40	1404538
Caelo	Ramsons herb	13072801	40	20130326
Caelo	Raspberry leaf	12362701	40	20121219
Caelo	Red poppy petals, cut	12008104	40	20120131
Caelo	Red-rose Flower	11299204	40	from supplier
Caelo	Red-rose petal	11304912	40	20111107
Caelo	Redwood, cut	12049604	40	20120229
Caelo	Restharrow root	12330001	40	20121127
Klenk	Restharrow root	6411B130404	40	20130507
Fagron	Resveratrol	24I18-B028	40	20241008*
Fagron	Resveratrol	24I18-B025	40	20241008*
Fagron	Resveratrol	24I18-B028	20	20241008*
Fagron	Resveratrol	24I18-B025	20	20241008*
Caelo	Rhubarb	12211906	40	20120827
Caelo	Rhubarb	13235213	40	20130822
Caelo	Rhubarb, powdered	11043818	60	1403280
Caelo	Rhubarb, powdered	16009901	60	9886
Euro OTC	Ribavirin	1304027-01	45	AR-16-FG-007485-01
Euro OTC	Ribavirin	1308001	45	20130902*
Euro OTC	Ribavirin	1604012	40	20160428*
Euro OTC	Ribavirin	1304027-02	40	20160429
Caelo	Ribwort plantain	12362902	40	20121220

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Rifampicin	152446	40	20150831*
Caelo	Rifaximin	161053	60	20160607*
Caelo	Rose hips peel	11301407	60	20111110
Klenk	Rose hips seed	7240A120402	60	20120404
Caelo	Rose hips with peel, cut	12064202	40	20120328
Caelo	Rose hips with peel, cut	11232204	40	20110919
Caelo	Rose mallow flower, cut	10244508	60	20100917
Caelo	Roselle	12007311	60	20120124
Caelo	Roselle	11036509	60	20110303
Bombastus	Rosemary leaf	23004436	30	20231017
Caelo	Rosemary leaf	14159601	60	20140617
Caelo	Rosemary leaf	23001738001	30	20231124
Klenk	Rosemary leaf	2261A131118	60	AR-15-FG-008499-01
Klenk	Ruscus rhizome, cut	7081B110301	60	20130131
Fagron	Rutoside trihydrate	13K12-B06-295483	60	20131204
Fagron	s-Acetylglutathione	22G01-B02-225858	40	20220706
Fagron	s-Acetylglutathione	23D21-B10-229486	40	20230809
Fagron	s-Acetylglutathione	22G01-B02-225858	20	20220706
Fagron	s-Acetylglutathione	23D21-B10-229486	20	20230809
Klenk	Saffron	0384A121022	40	20121114
Caelo	Sage leaf	11347503	40	20120102
Caelo	Sarsaparilla root, cut	10230402	60	20100909
Euro OTC	Selenium disulfide	1411011-02	40	20141211
Bombastus	Senna leaflet	24000491	30	20240130
Caelo	Senna leaflet	12273106	40	20120927
Caelo	Senna leaflet	23001268010	30	20230714
Caelo	Senna leaflet, powdered	11193307	120	pending
Caelo	Senna leaflet, powdered	12369908	40	1408079
Klenk	Senna leaflet, powdered	2334B130606	60	AR-15-FG-015212-01
Caelo	Senna pods, tinnevelly	12267605	40	20120921
Caelo	Senna pods, tinnevelly	11154404	40	20110607
Caelo	Senna pods, tinnevelly	13395106	40	20140106
EDQM	Sertaconazole nitrate	2.0	26	CRS
Caelo	Shepherd's purse	11328208	40	20111205
Caelo	Silica, colloidal anhydrous	181124	40	20180424*
Caelo	Silver nitrate	181276	40	20180716*
Caelo	Silver, colloidal	173615	40	20180312*
Caelo	Silverweed	11328105	40	20111130
Galke	Silverweed	22840	40	from supplier
Fagron	Simvastatin	24D29-B07-002224	40	20240730
Fagron	Simvastatin	24H01-B12-002225	40	20240927
Fagron	Simvastatin	24D29-B07-002224	20	20240730
Fagron	Simvastatin	24H01-B12-002225	20	20240927
Euro OTC	Sodium alginate	2305007	40	20230720*
Euro OTC	Sodium alginate	2305007	20	20230720*
Fagron	Sodium alginate	14G22-B99-297091	60	20140813
Gatt-Koller	Sodium alginate	22J01179	40	20220714
Gatt-Koller	Sodium alginate	22J01179	20	20220714
Caelo	Sodium bromide	171191	40	20170510*
Caelo	Sodium carbonate decahydrate	173613	40	20180115*
Gatt-Koller	Sodium carbonate decahydrate	23J00898	37	20230516
Gatt-Koller	Sodium carbonate decahydrate	23J00898	28	20230516
Caelo	Sodium carbonate monohydrate	16310205	40	20161221
Merck KGaA	Sodium diphosphate decahydrate	K55034491332	40	not required
Fagron	Sodium fusidate	23A04-B10-219743	40	20230209

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Fagron	Sodium fusidate	23F12-B05-22913	40	20230705
Fagron	Sodium fusidate	23A04-B10-219743	20	20230209
Fagron	Sodium fusidate	23F12-B05-22913	20	20230705
Audor	Sodium hyaluronate	AP30101404H	60	20141203
Audor	Sodium hyaluronate	AP30101702H	40	1802037
Caelo	Sodium hyaluronate	172347	40	20171004*
Euro OTC	Sodium hyaluronate	L1302028-01	40	1403532
Euro OTC	Sodium hyaluronate	L1302028-01	60	20130314
Kraeber & ...	Sodium hyaluronate	3462	40	20180723
Kraeber & ...	Sodium hyaluronate	3829	40	2104160
Kraeber & ...	Sodium hyaluronate	3897	40	20200408
Caelo	Sodium hydrocarbonate	23002402	40	20230919*
Caelo	Sodium hydrocarbonate	23002402	20	20230919*
Euro OTC	Sodium hydrocarbonate	1807021-01	40	20180725
Euro OTC	Sodium hydrocarbonate	2202008	40	20220317*
Euro OTC	Sodium hydrocarbonate	2302009	40	20230309*
Euro OTC	Sodium hydrocarbonate	2306010	40	20230718*
Euro OTC	Sodium hydrocarbonate	2202008	20	20220317*
Euro OTC	Sodium hydrocarbonate	2302009	20	20230309*
Caelo	Sodium iodide	161701	40	20160706*
Caelo	Sodium methyl-4-hydroxybenzoate	15358708	40	AR-16-FG-015095-01
Caelo	Sodium methyl-4-hydroxybenzoate	15358708	40	20151127
Caelo	Sodium methyl-4-hydroxybenzoate	15358709	40	20151127
Caelo	Sodium methyl-4-hydroxybenzoate	15358713	40	20151127
Caelo	Sodium methyl-4-hydroxybenzoate	170519	40	20170308*
Caelo	Sodium methyl-4-hydroxybenzoate	191439	40	20190628*
Caelo	Sodium monohydrogenphosphate dodecahydrate	22000404	40	20220211*
Caelo	Sodium monohydrogenphosphate dodecahydrate	22001508	40	20220531
Caelo	Sodium monohydrogenphosphate dodecahydrate	22002975	40	20220930*
Caelo	Sodium monohydrogenphosphate dodecahydrate	23002592	40	20231024*
Caelo	Sodium monohydrogenphosphate dodecahydrate	24000747	40	20240507*
Caelo	Sodium monohydrogenphosphate dodecahydrate	22000404	20	20220211*
Caelo	Sodium monohydrogenphosphate dodecahydrate	22001508	20	20220531
Caelo	Sodium monohydrogenphosphate dodecahydrate	22002975	20	20220930*
Caelo	Sodium monohydrogenphosphate heptahydrate	12109002	40	20120424
Caelo	Sodium monohydrogenphosphate heptahydrate	21003087	40	20210927*

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Sodium monohydrogenphosphate heptahydrate	21003087	20	20210927*
Caelo	Sodium nitrate	11045910	40	20110225
Caelo	Sodium nitrite	171360	30	20170522*
Euro OTC	Sodium sulfate, anhydrous	1801046-01	40	20180202
Caelo	Sodium thiosulfate	181648	40	20180712*
Caelo	Softisan® 601	13296104	40	1403144
Caelo	Softisan® 601	14099604	40	1504720
Caelo	Softisan® 601	15184905	60	20150611
Caelo	Softisan® 601	162364	40	20160823*
Caelo	Softisan® 601	162364	40	20160823*
Caelo	Softisan® 601	172178	40	20170817*
Caelo	Softisan® 601	20003054001	40	20201001
Caelo	Solanum dulcamara stems, cut	10375602	40	20110113
Caelo	Solanum dulcamara stems, cut	13254305	40	20130806
Caelo	Sour cherry stems, cut	12042302	40	1503570
Caelo	Spearmint leaf	12133906	40	20120516
Sigma-Aldrich	Stannous chloride dihydrate	K54805315247	40	not required
Caelo	Star anise	11314104	10	20111121
Caelo	Star anise, cut	12226301	60	pending
Caelo	Star anise, cut	13041401	40	1403709
Caelo	Star anise, cut	15329302	60	AR-16-FG-004770-01
Caelo	Stemless carline root	12163702	40	20120628
Caelo	Stemless carline root	12232802	40	20120822
Caelo	Strawberry leaf	11117903	40	20110428
Klenk	Strawberry leaf	2031B110224	40	20110304
Klenk	Strawberry leaf	2031B120925	40	20121005
Caelo	Sulfamerazine	10218403	30	20100914
Fagron	Sulfamethoxazole	22H23-B16-225919	40	20220909
Fagron	Sulfamethoxazole	22H23-B16-225919	20	20220909
Caelo	Sweet woodruff herb	10375812	30	20110114
Caelo	Talcum	22002768	40	20220928*
Euro OTC	Talcum	2204002	40	20220511*
Otto Fischar	Talcum	90841/1	40	from supplier
Caelo	Thalidomide	13395704	60	20140207
Caelo	Thalidomide	162703	40	20160929*
Caelo	Thalidomide	15276711	40	1704508
Caelo	Thalidomide	172100	40	20170821*
Caelo	Thalidomide	182496	40	20181022*
Fagron	Thalidomide	14E27B04295348	60	1503608
Fagron	Thalidomide	15A13-B01-312230	40	1704509
LGC Standa...	THCA-A	1457348	30	20240417
Fagron	Theacrine	24I18-B028	40	20241011*
Fagron	Theacrine	24I14-B018	40	20241011*
Fagron	Theophylline-ethylenediamine	19C04-B04-363517	40	20190823
Fagron	Theophylline-ethylenediamine	20J13-F05-375387	40	20201207
Caelo	Theriac	12289307	40	1405122
Caelo	Theriac	13407301	40	1410336
Klenk	Theriac	13816	60	1705088
Fagron	Thiamine nitrate	15A30-B06-309069	60	AR-16-FG-005855-01
Bombastus	Thyme	23005529	30	20231213
Caelo	Thyme	11345004	60	20111213
Caelo	Thyme	22003890005	30	20230622
Galke	Thyme	21932	40	from supplier
Euro OTC	Titanium dioxide	1708015-01	40	20170822

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
USP	Tobramycin	M0M058	40	CRS
Caelo	Tonka beans	12145101	40	20120604
Caelo	Tormentil	12040708	40	1403487
Caelo	Tormentil	12013103	40	1403048
Caelo	Tormentil	12040715	40	1403710
Caelo	Tormentil	13220502	40	1403049
Caelo	Tormentil	14360103	60	1606520
Klenk	Tormentil	6914B120112	40	20120118
Caelo	Tragacanth	13277804	60	1507149
Caelo	Tragacanth	15085602	60	20150410
Caelo	Tragacanth	15379906	60	20151124
Caelo	Tragacanth	16110802	60	AR-17-FG-007533-01
Caelo	Tribromophenol bismuth	18144202	40	20180706
Euro OTC	Tricalcium phosphate	1206002-01	40	1402298
Fagron	Trimethoprim	21J11-B07-219183	40	20220125
Fagron	Trimethoprim	23B17-B03-232012	40	20230322
Fagron	Trimethoprim	21J11-B07-219183	20	20220125
Fagron	Trimethoprim	23B17-B03-232012	20	20230322
Caelo	Turmeric rhizome	11160403	60	20110628
Caelo	Turmeric rhizome	12136503	40	1405295
Caelo	Turmeric rhizome	13360202	40	1411363
Caelo	Turmeric, javanese	12185605	40	1403465
Caelo	Turmeric, javanese	12319206	40	20121130
Caelo	Turmeric, javanese	13262904	40	20130926
Kräuter Schulte	Twotoothed achyranthes root, cut	45053	40	from supplier
Audor	Uridine	APIB1600169AU	40	20170711
Audor	Uridine	APIB160018211AU	40	20161118
Fagron	Uridine	11G07-N04	60	1402481
Fagron	Uridine	13K18-B31-288497	60	20131129
Caelo	Valerian root, cut	12033809	40	20120228
Caelo	Valerian root, powdered	12138005	40	1403809
Caelo	Valerian root, powdered	12138008	40	1508496
Caelo	Valerian root, powdered	13113204	60	pending
Caelo	Verbena herb	12187602	40	20120719
Klenk	Verbena herb	4651B120611	40	20121123
Fagron	Vinpocetine	20240501	40	20240512*
Fagron	Vinpocetine	20240501	20	20240512*
Euro OTC	Vitamin A acetate	2303019	40	20230414*
Euro OTC	Vitamin A acetate	2303019	20	20230414*
Caelo	Walnut bark	11325603	40	20111124
Caelo	Walnut leaf	11103007	40	1403091
Caelo	White deadnettle flower	11371604	40	20120103
Caelo	White mustard seed	13064301	40	pending
Caelo	White mustard seed	13380501	40	20140103
Caelo	White pepper	12294902	40	1403488
Caelo	White pepper	12294905	40	20121130
Caelo	White pepper	14010703	40	20140122
Caelo	Wild pansy	10291007	60	20101103
Caelo	Willow bark	12185204	40	20120730
Caelo	Willow herb	11347311	40	20111216
Caelo	Willowherb, small flowered	10326106	40	20101216
Caelo	Willowherb, small flowered	13355904	60	20140113
Klenk	Willowherb, small flowered	4721A140203	60	20140219
Caelo	Wormwood	12355801	40	20121211
Dr. Behr	Yam root extract	WE14020005-05	40	pending
Caelo	Yarrow flower	12267703	40	20120921
Caelo	Yellow chaste weed	11293101	40	20111028
Caelo	Zedoary root	12125301	40	20120522
Caelo	Zedoary root, powdered	12344601	40	1403489

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra	Certificate
Caelo	Zedoary root, powdered	13165501	40	pending
Caelo	Zedoary root, powdered	14249001	60	20141008
Caelo	Zinc oxide	14038101	40	20140205
Caelo	Zinc oxide-talcum powder mixture 1:1	181487	40	20180702*

*The spectra were taken from a part of the same sample which the supplier used for its analysis (identity, purity, content). In this case the manufacturer certificates proof the identity and quality of the sample from those the spectra descend.

Appendix C: Additional validation samples (*Type C*)

Spectra for substances from the field which cannot be identified with this model also enter the validation. In this manner, it is verified that the model also rejects unknown substances. The spectra for these samples were recorded by *Apo-Ident* customers. They belong to *Type C*. The information provided by the customer regarding the manufacturer and batch number is taken over by *HiperScan GmbH* to a large extent unchecked.

The samples originate from 7975 batches. From these, 19 047 spectra were recorded. The spectra recorded on independent samples of substances from the field which can be identified with the model are listed respectively in the section *Type C* for the individual substances and do not appear again elsewhere in this list.

0 A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

Supplier	Substance	Batch	Spectra
Fagron	(R,S)-epinephrine hydrochloride	14A22-B05	1
Fagron	(R,S)-epinephrine hydrochloride	2021503	1
Fagron	(R,S)-epinephrine hydrochloride	10022015E	1
Fagron	(R,S)-epinephrine hydrochloride	14a22-B05	1
Fagron	(R,S)-epinephrine hydrochloride	16H23-B98-325052	1
Dermapharm	8-quinolinol sulfate monohydrate	140804	1
Dermapharm	8-quinolinol sulfate monohydrate	100804	1
Fagron	8-quinolinol sulfate monohydrate	10F01-N15	1
Fagron	8-quinolinol sulfate monohydrate	11L08-N07	2
Fagron	8-quinolinol sulfate monohydrate	11/09-N09	1
Fagron	8-quinolinol sulfate monohydrate	11L19-N14	1
Fagron	8-quinolinol sulfate monohydrate	13/21-N23	1
Fagron	8-quinolinol sulfate monohydrate	13D24-N11	1
Fagron	8-quinolinol sulfate monohydrate	13G10-N06	1
Fagron	8-quinolinol sulfate monohydrate	12A04-N05	1
Fagron	8-quinolinol sulfate monohydrate	11I09-N09	1
Fagron	8-quinolinol sulfate monohydrate	13A04-N05	1
Fagron	8-quinolinol sulfate monohydrate	12D26-N04	1
Fagron	8-quinolinol sulfate monohydrate	12H21-N08	1
Fagron	8-quinolinol sulfate monohydrate	13032014C	1
Dermapharm	8-quinolinol sulfate monohydrate	120905	1
siehe WE-Prüfprotokoll	8-quinolinol sulfate monohydrate	96/09	1

A

Supplier	Substance	Batch	Spectra
Caelo	Abrotani herb, cut	2091305	1
Klenk	Abrotani herb, cut	21081301	1
Klenk	Abrotani herb, cut	26011403	1
Nachprüfung	Abrotani herb, cut	3451A070919	1
Noweda	Abrotani herb, cut	3451A120312	19
Bombastus	Acorus root	276260	2
Bombastus	Acorus root	224114	1
Bombastus	Acorus root	281692	2
Bombastus	Acorus root	277958	1
Bombastus	Acorus root	274159	1
Caelo	Acorus root	13127801	1
Caelo	Acorus root	284875	2
Klenk	Acorus root	B130807	1
Caelo	Acorus root	12066501	1
Aurica/Phönix	Acorus root, peeled	150649	1
Bahnhof-Apotheke	Acorus root, peeled	17-121107	1
Bombastus	Acorus root, peeled	267365	1
Bombastus	Acorus root, peeled	274159	3
Caelo	Acorus root, peeled	15061202	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Acorus root, peeled	24081203	1
Caelo	Acorus root, peeled	12056703	1
Caelo	Acorus root, peeled	12066501	7
Caelo	Acorus root, peeled	12066502	1
Caelo	Acorus root, peeled	28121205	1
Caelo	Acorus root, peeled	8031306	1
Caelo	Acorus root, peeled	12295901	1
Caelo	Acorus root, peeled	6701B130103	21
Caelo	Acorus root, peeled	12295904	4
Caelo	Acorus root, peeled	7061302	1
Caelo	Acorus root, peeled	313060	1
Caelo	Acorus root, peeled	12295903	1
Caelo	Acorus root, peeled	12275602	7
Caelo	Acorus root, peeled	241013010	1
Caelo	Acorus root, peeled	12275604	2
Caelo	Acorus root, peeled	12056701	1
Caelo	Acorus root, peeled	12295902	4
Caelo	Acorus root, peeled	12239008	1
Caelo	Acorus root, peeled	12275604-3544411013	1
Caelo	Acorus root, peeled	13101306	1
Galke	Acorus root, peeled	18944	1
Gehe	Acorus root, peeled	6701B130807	9
Klenk	Acorus root, peeled	6701B150407	1
Klenk	Acorus root, peeled	106212173	1
Klenk	Acorus root, peeled	6701B120427	7
Klenk	Acorus root, peeled	6701B120817	6
Klenk	Acorus root, peeled	6701B130870	1
Klenk	Acorus root, peeled	6711B110606	1
Klenk	Acorus root, peeled	4797362	1
Klenk	Acorus root, peeled	6701b120301	1
Klenk	Acorus root, peeled	6701b130103	1
Klenk	Acorus root, peeled	6701B120301	3
Caelo	Agarikon	11024502	1
Berkel AHK	Agnus castus fruit	14194401	4
Caelo	Agnus castus fruit	11026309	1
Caelo	Agnus castus fruit	12016909	4
Caelo	Agnus castus fruit	12016902	1
Caelo	Agnus castus fruit	12016908	1
Caelo	Agnus castus fruit	12274010	10
Caelo	Agnus castus fruit	12274008	1
Caelo	Agnus castus fruit	12274009	3
Caelo	Agnus castus fruit	12274014	1
Caelo	Agnus castus fruit	13193401	2
Caelo	Agnus castus fruit	13193403	1
Caelo	Agnus castus fruit	1513546	1
Caelo	Agnus castus fruit	13193407	1
Caelo	Agnus castus fruit	13193410	2
Caelo	Agnus castus fruit	14194408	1
Caelo	Agnus castus fruit	15318702	1
Caelo	Agnus castus fruit	15318705	1
Caelo	Agnus castus fruit	15318718	1
Caelo	Agnus castus fruit	9245308	1
Caelo	Agnus castus fruit	12274002	1
Caelo	Agnus castus fruit	13193406	1
Caelo	Agnus castus fruit	15065105	1
Caelo	Agnus castus fruit	11026318	1
Caelo	Agnus castus fruit	12274013	2
Caelo	Agnus castus fruit	3413A-03015	1
Caelo	Agnus castus fruit	80175158	2
Caelo	Agnus castus fruit	12016905	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Agnus castus fruit	13193404	1
Gutenberg-Apotheke	Agnus castus fruit	61765	1
Klenk	Agnus castus fruit	A120803	1
Klenk	Agnus castus fruit	7110N090701	1
Klenk	Agnus castus fruit	A110614	3
Klenk	Agnus castus fruit	7110A120803	1
Klenk	Agnus castus fruit	7110A110614	2
Klenk	Agnus castus fruit	A130613	1
Klenk	Agnus castus fruit	7110N150121	1
Klenk	Agnus castus fruit	7110A130613	1
Klenk	Agnus castus fruit	12274007	3
Sanacorp	Agnus castus fruit	12274006	3
Caelo	Agnus castus fruit	12274003	4
Caelo	Agnus castus fruit	12274012	1
Alliance	Agrimony	11374004	5
Anzag 05.12.12	Agrimony	11374002	3
Caelo	Agrimony	10325502	2
Caelo	Agrimony	10325505	1
Caelo	Agrimony	12382903	1
Caelo	Agrimony	1137407	1
Caelo	Agrimony	11374005	2
Caelo	Agrimony	12382901	3
Caelo	Agrimony	3481-A-110324	1
Caelo	Agrimony	11374006	6
Celo	Agrimony	11374003	1
Galke	Agrimony	2002	1
Herbasinica	Agrimony	11374007	1
Klenk	Agrimony	3481C120508	1
Noweda	Agrimony	9300106	1
Noweda	Agrimony	10325503	2
Sino Phyto	Agrimony	12382905	5
Alfred Galke	Alchemilla	20921	1
Caelo	Alchemilla	13141105	3
Anzag ek: 6,39 11…	Alchemilla	11182806	6
Bombastus	Alchemilla	279070	5
Bahnhof-Apotheke	Alchemilla	17-121107	1
Bombastus	Alchemilla	272021	5
Bombastus	Alchemilla	276173	3
Bombastus	Alchemilla	278889	1
Bombastus	Alchemilla	282032	2
Bombastus	Alchemilla	14066007	1
Bombastus	Alchemilla	521203995	1
Bombastus	Alchemilla	266404	1
Bombastus	Alchemilla	231013B	1
Caelo	Alchemilla	1100912	1
Caelo	Alchemilla	11002906	5
Caelo	Alchemilla	11182801	3
Caelo	Alchemilla	11182804	3
Caelo	Alchemilla	1406211616	1
Caelo	Alchemilla	11182807	2
Caelo	Alchemilla	21081203	1
Caelo	Alchemilla	11182805	1
Caelo	Alchemilla	11063605	1
Caelo	Alchemilla	11182808	1
Caelo	Alchemilla	12153301	3
Caelo	Alchemilla	8121201	1
Caelo	Alchemilla	12153303	7
Caelo	Alchemilla	12153305	25
Caelo	Alchemilla	12153307	3
Caelo	Alchemilla	12342901	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Alchemilla	5041301	1
Caelo	Alchemilla	125306	1
Caelo	Alchemilla	H-040513-2	1
Caelo	Alchemilla	13141103	36
Caelo	Alchemilla	2081304	1
Caelo	Alchemilla	intch:318080	1
Caelo	Alchemilla	3613M01616	1
Caelo	Alchemilla	13091304	1
Caelo	Alchemilla	13141106	8
Caelo	Alchemilla	9011405	1
Caelo	Alchemilla	27011401	1
Caelo	Alchemilla	14066002	2
Caelo	Alchemilla	14066008	1
Caelo	Alchemilla	15147002	2
Caelo	Alchemilla	1118206	1
Caelo	Alchemilla	1213309	1
Caelo	Alchemilla	1215305	2
Caelo	Alchemilla	131411002	1
Caelo	Alchemilla	13141102	6
Caelo	Alchemilla	5013I1616	1
Caelo	Alchemilla	13141101	7
Caelo	Alchemilla	1215309	1
Caelo	Alchemilla	13141103-3382319003	1
Caelo	Alchemilla	13141103-3400310161	1
Caelo	Alchemilla	13141103-3456311103	1
Caelo	Alchemilla	13141106-3545412081	1
Galke	Alchemilla	21141	1
Galke	Alchemilla	22291	1
Galke	Alchemilla	19835	1
Gehe	Alchemilla	1341102	1
Klenk	Alchemilla	3501C121105	4
Hepart AG	Alchemilla	21963	3
Hepart AG	Alchemilla	B-698kbA	1
Ichtyol/Phönix	Alchemilla	13141107	3
Klenk	Alchemilla	3501B100428	1
Klenk	Alchemilla	3501B090417	1
Klenk	Alchemilla	3501A110301	3
Noweda	Alchemilla	12153302	13
Caelo	Alchemilla	14066003	1
Sanacorp	Alchemilla	12153309	14
Caelo	Alchemilla	12153306	5
Fagron	Alchemilla	11182802	1
Wolf	Alchemilla	E-822	1
Wolf	Alchemilla	B-698	2
Wolf	Alchemilla	23187	4
Wolf	Alchemilla	p931	1
Caelo	Alchemilla alpina herb, cut	12147202	3
Caelo	Alchemilla alpina herb, cut	12147205	2
Caelo	Alchemilla alpina herb, cut	12147203	1
Caelo	Alchemilla alpina herb, cut	1214204	1
Caelo	Alchemilla alpina herb, cut	12147203-3470312131	1
Caelo	Alchemilla alpina herb, cut	11063608	1
Caelo	Alchemilla alpina herb, cut	12147206	3
Klenk	Almonds, bitter, whole	40A161028	13
Klenk	Almonds, bitter, whole	40A-150904	2
Klenk	Almonds, bitter, whole	40A161206	8
Apotheke Bühlau	Almonds, bitter, whole	267467	2
Bombastus	Almonds, bitter, whole	275001	3
Bombastus	Almonds, bitter, whole	275600	1
Bombastus	Almonds, bitter, whole	283369	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Almonds, bitter, whole	284978	1
Bombastus	Almonds, bitter, whole	297921	1
Bombastus	Almonds, bitter, whole	304961	1
Bombastus	Almonds, bitter, whole	1700352	2
Bombastus	Almonds, bitter, whole	17000353	1
Bombastus	Almonds, bitter, whole	306048	1
Bombastus	Almonds, bitter, whole	303218	2
Bombastus	Almonds, bitter, whole	305322	2
Bombastus	Almonds, bitter, whole	275601	1
Bombastus	Almonds, bitter, whole	267529	1
Caelo	Almonds, bitter, whole	12239604	1
Caelo	Almonds, bitter, whole	13242001	1
Caelo	Almonds, bitter, whole	5121301	1
Caelo	Almonds, bitter, whole	15193103	1
Euro OTC	Almonds, bitter, whole	290973	2
Fagron	Almonds, bitter, whole	40A161005	5
Caelo	Almonds, bitter, whole	16221202	1
Klenk	Almonds, bitter, whole	40A150904	18
Klenk	Almonds, bitter, whole	40A120924	4
Klenk	Almonds, bitter, whole	40A121010	11
Klenk	Almonds, bitter, whole	40A111004	1
Klenk	Almonds, bitter, whole	40A111117	7
Klenk	Almonds, bitter, whole	40A140908	19
Klenk	Almonds, bitter, whole	40A0130909	1
Klenk	Almonds, bitter, whole	40A130909	9
Klenk	Almonds, bitter, whole	40A150905	1
Klenk	Almonds, bitter, whole	40A0161005	1
Anzag 22.03.13 ek:…	Aloes, cape, powdered	12232102	1
Caelo	Aloes, cape, powdered	11132115	1
Caelo	Aloes, cape, powdered	12183007	1
Caelo	Aloes, cape, powdered	12183009	3
Caelo	Aloes, cape, powdered	14065905	1
Caelo	Aloes, cape, powdered	15206501	1
Caelo	Aloes, cape, powdered	12183008	1
Caelo	Aloes, cape, powdered	12183001	1
Caelo	Aloes, cape, powdered	14065906	1
Caelo	Aloes, cape, powdered	11132116	2
Caelo	Aloes, cape, powdered	15206514	1
Caelo	Aloes, cape, powdered	15206516	1
Caelo	Aloes, cape, powdered	11132116	1
Caelo	Aloes, cape, powdered	12183013	3
Caesar / Gehe	Aloes, cape, powdered	15206507	2
Klenk	Aloes, cape, powdered	24A160620	1
Caelo	Aloes, cape, powdered	16202410	1
Caelo	Aluminium potassium sulfate…	14263804	1
Alliance Health	Aluminium potassium sulfate…	13025401	3
Alliance Healthcare	Aluminium potassium sulfate…	13025404	1
Anzag	Aluminium potassium sulfate…	1218441	1
Caelo	Aluminium potassium sulfate…	1218411	1
Caelo	Aluminium potassium sulfate…	12022444	1
Caelo	Aluminium potassium sulfate…	12022404	1
Caelo	Aluminium potassium sulfate…	510211092	1
Caelo	Aluminium potassium sulfate…	11017211	1
Caelo	Aluminium potassium sulfate…	12022406	2
Caelo	Aluminium potassium sulfate…	12184401	2
Caelo	Aluminium potassium sulfate…	12184407	3
Caelo	Aluminium potassium sulfate…	504311092	1
Caelo	Aluminium potassium sulfate…	90033229	1
Caelo	Aluminium potassium sulfate…	12144605	4
Caelo	Aluminium potassium sulfate…	12184408	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Aluminium potassium sulfate...	12144607	2
Caelo	Aluminium potassium sulfate...	12239102	2
Caelo	Aluminium potassium sulfate...	13025401	3
Caelo	Aluminium potassium sulfate...	12184411	1
Caelo	Aluminium potassium sulfate...	2713Q1092	1
Caelo	Aluminium potassium sulfate...	13025404	3
Caelo	Aluminium potassium sulfate...	15172501	1
Caelo	Aluminium potassium sulfate...	12184401	1
Caelo	Aluminium potassium sulfate...	12144602	1
Caelo	Aluminium potassium sulfate...	12184406	2
Caelo	Aluminium potassium sulfate...	11254805	1
Caelo	Aluminium potassium sulfate...	11218611	2
Caelo	Aluminium potassium sulfate...	12184402	3
Caelo	Aluminium potassium sulfate...	13098702	1
Caelo	Aluminium potassium sulfate...	12184407	5
Caelo	Aluminium potassium sulfate...	12022409	1
Caelo	Aluminium potassium sulfate...	12022401	1
Caelo	Aluminium potassium sulfate...	12022406	1
Caesar/Noweda	Aluminium potassium sulfate...	12184411	2
Euro OTC	Aluminium potassium sulfate...	1004046-02	1
Fagron	Aluminium potassium sulfate...	A1-063-Al	1
Fagron	Aluminium potassium sulfate...	12/24-M02	1
Fagron	Aluminium potassium sulfate...	103638	1
Fagron	Aluminium potassium sulfate...	A1-063-AL	1
Fagron	Aluminium potassium sulfate...	13D08-N01	1
Caelo	Aluminium potassium sulfate...	12|24-M03	1
Fagron	Aluminium potassium sulfate...	13D29-N04	1
Sanacorp	Aluminium potassium sulfate...	12184402	2
Caelo	Aluminium potassium sulfate...	12144603	1
Fagron	Aluminium potassium sulfate...	12I24-M03	1
Caesar/Noweda	American liverwort, cut	11254608	1
Caelo	Ammonium chloride	10176319	2
Caelo	Ammonium chloride	12240302	4
Caelo	Ammonium chloride	12356101	3
Caelo	Ammonium chloride	10176309	1
Euro OTC	Ammonium chloride	1212017-01	2
Euro OTC	Ammonium chloride	1303029-01	1
Euro OTC	Ammonium chloride	1203029-01	1
Euro OTC	Ammonium chloride	512A-01104	1
	Amphetamine sulfate	22I08-F02-383423	1
Bombastus	Amphetamine sulfate	C18H28N2O4S	1
Caelo	Amphetamine sulfate	12I24-N03	1
Caelo	Amphetamine sulfate	13344609	1
Caelo	Amphetamine sulfate	15193204	3
Caelo	Amphetamine sulfate	16153903	4
Caelo	Amphetamine sulfate	16153909	1
Caelo	Amphetamine sulfate	1807171	1
Caelo	Amphetamine sulfate	70325	124
Caelo	Amphetamine sulfate	17K03-B01	1
Caelo	Amphetamine sulfate	18186903	1
Caelo	Amphetamine sulfate	16143001	1
Caelo	Amphetamine sulfate	20004272011	2
Caelo	Amphetamine sulfate	16153902	1
Caelo	Amphetamine sulfate	lot067002	1
Caelo	Amphetamine sulfate	15L01-B05	3
Caelo	Amphetamine sulfate	200004272001	1
Caelo	Amphetamine sulfate	200004272009	1
Caelo	Amphetamine sulfate	2004272001	1
Caelo	Amphetamine sulfate	22003072004	1
Caelo	Amphetamine sulfate	16153905	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Amphetamine sulfate	12B06-N013	1
Caesar & Loretz GmbH	Amphetamine sulfate	16153901	1
Caesar & Loretz GmbH	Amphetamine sulfate	20004272001	5
Caesar & Loretz GmbH	Amphetamine sulfate	20004272002	2
Caesar & Loretz GmbH	Amphetamine sulfate	22003072002	1
Caesar & Loretz Gm…	Amphetamine sulfate	22003072003	3
Fagron	Amphetamine sulfate	12E11-N06	2
Fagron	Amphetamine sulfate	F001287	1
Fagron	Amphetamine sulfate	13B11-N04	2
Fagron	Amphetamine sulfate	13D09-N03	1
Fagron	Amphetamine sulfate	88689	2
Fagron	Amphetamine sulfate	96200	2
Fagron	Amphetamine sulfate	15L01-B05-315291	6
Fagron	Amphetamine sulfate	16A29-B03	11
Fagron	Amphetamine sulfate	16A29B03318744	1
Fagron	Amphetamine sulfate	15l01-b05-315292	1
Fagron	Amphetamine sulfate	324577	2
Fagron	Amphetamine sulfate	315291	1
Fagron	Amphetamine sulfate	16a29-B03-319156	1
Fagron	Amphetamine sulfate	17K03-B01-344122	3
Fagron	Amphetamine sulfate	19H05-B01-363346	4
Fagron	Amphetamine sulfate	B01_3655801	1
Fagron	Amphetamine sulfate	78012	1
Fagron	Amphetamine sulfate	1117I-03361	1
Fagron	Amphetamine sulfate	16K08-B04-336362	1
Fagron	Amphetamine sulfate	16A29-B03-318743	6
Fagron	Amphetamine sulfate	16A29_B03_318744	1
Fagron	Amphetamine sulfate	19H05-B01-365582	3
Fagron	Amphetamine sulfate	11/01-N01	1
Fagron	Amphetamine sulfate	16A29-B03-328317	6
Fagron	Amphetamine sulfate	2213Q-03361	1
Fagron	Amphetamine sulfate	16A29-B03-328318	1
Fagron	Amphetamine sulfate	11D04-N13	1
Fagron	Amphetamine sulfate	13J18B40	1
Fagron	Amphetamine sulfate	16A29-B03-324578	4
Fagron	Amphetamine sulfate	19H05-B01-365581	2
Fagron	Amphetamine sulfate	16a29-b03-318744	2
Fagron	Amphetamine sulfate	12/24N-03	1
Fagron	Amphetamine sulfate	13G08-N11	3
Fagron	Amphetamine sulfate	13J18-B40	1
Fagron	Amphetamine sulfate	14E19-B09	2
Fagron	Amphetamine sulfate	19H05-B01-364791	1
Fagron	Amphetamine sulfate	20I18-F06	2
Fagron	Amphetamine sulfate	12B06-N13	2
Fagron	Amphetamine sulfate	15L01-B05-315292	7
Fagron	Amphetamine sulfate	15L01-B05-315290	1
Fagron	Amphetamine sulfate	16K08B04336362	1
Fagron	Amphetamine sulfate	19H05-B01-363347	1
Fagron	Amphetamine sulfate	19H05-B01-3633407	1
Fagron	Amphetamine sulfate	13J18-B40-290538	1
Fagron	Amphetamine sulfate	14E19-B09-304502	2
Fagron	Amphetamine sulfate	16K08-B04-336361	2
Fagron	Amphetamine sulfate	16K08-B04	1
Fagron	Amphetamine sulfate	19H05-B01-363345	4
Fagron	Amphetamine sulfate	19H05-B01	1
Gatt Koller/Herba	Amphetamine sulfate	942/03130814	1
Gatt-Koller	Amphetamine sulfate	18.03969	1
Gatt-Koller	Amphetamine sulfate	22J01850	1
Th. Geyer	Amphetamine sulfate	67043P-180924-1	1
Th. Geyer	Amphetamine sulfate	70325P-190404-1	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Th. Geyer	Amphetamine sulfate	57043	1
Noweda	Amphetamine sulfate	16A29-B03-318744	3
Noweda 7.8.19	Amphetamine sulfate	70325P-190808-1	1
Fagron	Amphetamine sulfate	14E19-B09-294572	1
Phoenix	Amphetamine sulfate	16A29-B03-328317	1
Phönix	Amphetamine sulfate	13B11N04	1
Phönix	Amphetamine sulfate	16a29-b03-328317	1
Fagron	Amphetamine sulfate	19h05b01365581	1
Sanacorp	Amphetamine sulfate	12/24-N03	1
Th. Geyer	Amphetamine sulfate	PH10051	3
Th. Geyer	Amphetamine sulfate	LOT067043	1
Th. Geyer	Amphetamine sulfate	20170808-03361	1
Th. Geyer	Amphetamine sulfate	LOT:070325	1
Th. Geyer	Amphetamine sulfate	6703	1
Th. Geyer	Amphetamine sulfate	LOT070325	2
Th. Geyer	Amphetamine sulfate	21082013B	1
Th. Geyer	Amphetamine sulfate	67043	96
Th. Geyer	Amphetamine sulfate	70525	1
Th. Geyer	Amphetamine sulfate		1
Th. Geyer	Amphetamine sulfate	67002	51
Th. Geyer	Amphetamine sulfate	618E-03361	1
-	Angelica root	130924	1
Bombastus	Angelica root	275879	1
Aurica/Phönix	Angelica root	520800638	1
Bombastus	Angelica root	272895	1
Bombastus	Angelica root	274128	2
Bombastus	Angelica root	269775	2
Bombastus	Angelica root	272954	1
Bombastus	Angelica root	270117	1
Bombastus	Angelica root	281280	7
Bombastus	Angelica root	301768	1
Bombastus	Angelica root	290309	1
Bombastus	Angelica root	307041	4
Bombastus	Angelica root	291848	1
Bombastus	Angelica root	295085	2
Bombastus	Angelica root	305460	1
Bombastus	Angelica root	275878	1
Caelo	Angelica root	11093304	1
Caelo	Angelica root	12168703	2
Caelo	Angelica root	12080403	1
Caelo	Angelica root	30011302	1
Caelo	Angelica root	269740	1
Caelo	Angelica root	6081B130109	7
Caelo	Angelica root	10071306	1
Caelo	Angelica root	Int.Ch:318090	1
Caelo	Angelica root	12350705	1
Caelo	Angelica root	5091303	1
Caelo	Angelica root	15101304	1
Caelo	Angelica root	21011402	1
Caelo	Angelica root	12080412	1
Caelo	Angelica root	28101402	1
Caelo	Angelica root	13041711	1
Caelo	Angelica root	17053302	1
Caelo	Angelica root	12168701	3
Caelo	Angelica root	12350703	9
Caelo	Angelica root	12350704	2
Caelo	Angelica root	15162604	2
Caelo	Angelica root	12168705	2
Caelo	Angelica root	14179506	2
Caelo	Angelica root	16128006	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Angelica root	285732	2
Caelo	Angelica root	16128002	3
Caelo	Angelica root	9030301	1
Caelo	Angelica root	303299	1
Caelo	Angelica root	5162606	1
Caelo	Angelica root	17053301	1
Euro OTC	Angelica root	301767	3
gasser	Angelica root	950049	1
Gehe	Angelica root	285732	1
Bombastus	Angelica root	296334/1121115	1
Klenk	Angelica root	6081B130410	4
Klenk	Angelica root	17053308	1
Klenk	Angelica root	6081N120110	14
Klenk	Angelica root	6081n120110	1
Klenk	Angelica root	B130109	2
Klenk	Angelica root	6091B130109	1
Klenk	Angelica root	6081B130109	1
Klenk	Angelica root	6081B140918	2
Klenk	Angelica root	6081B130726	1
Klenk	Angelica root	6081B150701	7
Klenk	Angelica root		1
Klenk	Angelica root	6081B170601	4
Klenk	Angelica root	6085B120614	1
Klenk	Angelica root	6081b130109	2
Klenk	Angelica root	6082b130410	1
Caelo	Angelica root	17053304	2
Noweda	Angelica root	272720	2
Bombastus	Angelica root	278294	1
Bombastus	Angelica root	278757	4
Caelo	Angelica root	14178506	1
Sanacorp	Angelica root	277310	1
Klenk	Angelica root	6081B160908	1
Weltecke	Angelica root	38011111	1
AHD 10.02.17 EK.3,50	Aniseed	16200801	5
Anzag 06.04.2016	Aniseed	15398601	1
Caelo	Aniseed	1137033	1
Aurica	Aniseed	521302895	1
Bahnhof-Apotheke	Aniseed	7-120913	1
Berkel AHK	Aniseed	11374103	1
Berkel AHK	Aniseed	14194401	1
Bombastus	Aniseed	285778	2
Bombastus	Aniseed	309836	1
Bombastus	Aniseed	282917	2
Bombastus	Aniseed	289846	2
Bombastus	Aniseed	285777	1
Bombastus	Aniseed	305177	1
Caelo	Aniseed	13037805	11
Caelo	Aniseed	PrüfNr4913E-01530	1
Caelo	Aniseed	13333913	1
Caelo	Aniseed	11101202	3
Caelo	Aniseed	10081207	1
Caelo	Aniseed	11101201	1
Caelo	Aniseed	11101215	3
Caelo	Aniseed	11370303	13
Caelo	Aniseed	10247202	1
Caelo	Aniseed	4061301	1
Caelo	Aniseed	5061301	1
Caelo	Aniseed	13037804	7
Caelo	Aniseed	13037801	1
Caelo	Aniseed	5091304	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Aniseed	13037901	1
Caelo	Aniseed	12360801	1
Caelo	Aniseed	13037808	9
Caelo	Aniseed	13333903	4
Caelo	Aniseed	13333901	6
Caelo	Aniseed	13333902	9
Caelo	Aniseed	5121401	1
Caelo	Aniseed	13333906	3
Caelo	Aniseed	13333909	2
Caelo	Aniseed	13333910	4
Caelo	Aniseed	13333914	1
Caelo	Aniseed	13333916	1
Caelo	Aniseed	15046103	3
Caelo	Aniseed	15046106	1
Caelo	Aniseed	15049103	1
Caelo	Aniseed	16165303	1
Caelo	Aniseed	16165304	4
Caelo	Aniseed	16165302	1
Caelo	Aniseed	15398607	1
Caelo	Aniseed	161635305	1
Caelo	Aniseed	17045603	3
Caelo	Aniseed	17045601	1
Caelo	Aniseed	16165308	1
Caelo	Aniseed	17045609	4
Caelo	Aniseed	17045611	3
Caelo	Aniseed	11121705	1
Caelo	Aniseed	13037803	2
Caelo	Aniseed	13037809	12
Caelo	Aniseed	17045602	3
Caelo	Aniseed	15398605	7
Caelo	Aniseed	15046102	12
Caelo	Aniseed	111101213	1
Caelo	Aniseed	11101213	2
Caelo	Aniseed	15046101	5
Caelo	Aniseed	3314E-01530	1
Caelo	Aniseed	2215M-01530	1
Caelo	Aniseed	2916E-01530	1
Caelo	Aniseed	15283201	6
Caelo	Aniseed	11370301	10
Caelo	Aniseed	13333908	7
Caelo	Aniseed	11370308	3
Caelo	Aniseed	15398603	5
Caelo	Aniseed	16165306	5
Caelo	Aniseed		1
Caelo	Aniseed	11101203	6
Caelo	Aniseed	13037807	2
Caelo	Aniseed	11370302	4
Caelo	Aniseed	12226402	5
Caelo	Aniseed	140913a	1
Caelo	Aniseed	13333907	4
Caelo	Aniseed	1539805	1
Caelo	Aniseed	17045608	1
Caelo	Aniseed	15046109	5
Caelo	Aniseed	15046110	1
Caelo	Aniseed	13037808-3560412014	1
Caelo	Aniseed	16165305	6
Caelo	Aniseed	15398601I-301216/5	1
Caelo	Aniseed	15398602	5
Caelo	Aniseed	13333912	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz/Noweda	Aniseed	153986002	1
Fagron	Aniseed	11370304	7
galke	Aniseed	19654	1
Galke	Aniseed	21278	1
Galke	Aniseed	22274	1
Galke	Aniseed	23464	1
GALKE	Aniseed	29047	1
Gehe	Aniseed	10247203	1
Gutenberg-Apotheke	Aniseed	1333902	1
Hepart AG	Aniseed	B216346,kbA	1
Jenne	Aniseed	2700A131015	2
Klenk	Aniseed	212M-01530	1
Klenk	Aniseed	2700A110701	7
Klenk	Aniseed	2901311530	1
Klenk	Aniseed	2103311530	1
Klenk	Aniseed	3113Q01530	1
Klenk	Aniseed	2700A130527	15
Klenk	Aniseed	2700A160511	8
Klenk	Aniseed	2700A150810	2
Klenk	Aniseed	2700A170803	1
Klenk	Aniseed	2700A190107	1
Klenk	Aniseed	2700A-110701	1
Klenk	Aniseed	2700A120320	8
Klenk	Aniseed	2700a120320	1
Klenk	Aniseed	2700A150901	3
Klenk	Aniseed	2700A12107	1
Klenk	Aniseed	814Q01530	1
Klenk	Aniseed	Klenk2700A131015	1
Klenk	Aniseed	2700A140129	9
Klenk	Aniseed	2700A121107	1
Klenk	Aniseed	2700A150601	11
nachprüfung	Aniseed	C1246	1
Nachprüfung	Aniseed	5010U-01530	1
Caelo	Aniseed	13037802	9
Caelo	Aniseed	11101214	6
siehe Protokoll	Aniseed	sieheProtokoll	1
Wolf	Aniseed	215346	1
Wolf	Aniseed	B216346	14
Wolf	Aniseed	216346	1
Wolf	Aniseed	B-671	2
Wolf	Aniseed	B671	1
Wolf	Aniseed	L401F292b	4
Wolf	Aniseed	L401F1413	1
Caelo	Aniseed, pounded	12111304	1
Caelo	Aniseed, pounded	11242003	1
Caelo	Aniseed, pounded	4041302	1
Caelo	Aniseed, pounded	23041303	1
Caelo	Aniseed, pounded	15149702	1
Caelo	Aniseed, pounded	1314990	1
Caelo	Aniseed, pounded	12111303	3
Gahlke	Aniseed, pounded	21401	1
Gehe	Aniseed, pounded	13149903	1
Caelo	Aniseed, pounded	13149902	1
Caelo	Aniseed, pounded	12360803	2
Klenk	Aniseed, pounded	2706B100120	1
Aurica Naturheilmi…	Aniseed, powdered	521405796	1
Klenk	Aniseed, powdered	2704B110824	1
vedono	Aniseed, powdered	11306208	1
Caelo	Apple, cut	12227301	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Apple, cut	A120302	3
Caelo	Arnica flower	10207405	1
Caelo	Arnica flower	28071201	1
Caelo	Arnica flower	10081204	1
Caelo	Arnica flower	11259804	1
Caelo	Arnica flower	12227202	1
Caelo	Arnica flower	122227202	1
Caelo	Arnica flower	IntCh:212032	1
Caelo	Arnica flower	11285705	1
Caelo	Arnica flower	11259803	1
Caelo	Arnica flower	11285703	1
Caelo	Arnica flower	6112013A	1
Caelo	Arnica flower	12227203	1
Caelo	Arnica flower	1222702	1
Caelo	Arnica flower	11374105	1
Caelo	Arnica flower	11374103	1
Caelo	Arnica flower	11374101	2
Caelo	Arnica flower	11374102	2
Gehe	Arnica flower	11259801	2
Klenk	Arnica flower	1181B130605	1
Bombastus	Artichoke leaf	8202213593	1
Caelo	Artichoke leaf	12173302	3
Caelo	Artichoke leaf	12173304	3
Caelo	Artichoke leaf	12173307	6
Caelo	Artichoke leaf	2312I-03593	1
Caelo	Artichoke leaf	12173306	2
Caelo	Artichoke leaf	13037607	4
Caelo	Artichoke leaf	13037608	1
Caelo	Artichoke leaf	13037603	1
Caelo	Artichoke leaf	81232298	1
Caelo	Artichoke leaf	12173307-3260315072	1
Caelo	Artichoke leaf	13310706	1
Kenk / Phoenix	Artichoke leaf	1981B130111	3
Klenk	Artichoke leaf	B121025	2
Klenk	Artichoke leaf	1981B121025	2
Klenk	Artichoke leaf	1981B120413	1
Caelo	Ash leaf, cut	12225504	1
Caelo	Ash leaf, cut	12225502	1
Caelo	Ash leaf, cut	12225505	2
Klenk	Ash leaf, cut	5111A-01491	1
Caelo	Asparagus root, cut	13193302	1
Caelo	Asparagus root, cut	13193308	1
Caelo	Asparagus root, cut	15010802	1
Galke	Asparagus root, cut	20178	1
Caelo	Asparagus root, cut	13071002	1
Klenk	Asparagus root, cut	6151B100332	1
Klenk	Asplenium scolopendrium, cut	4451B091116	1
Klenk	Asplenium scolopendrium, cut	4451B120605	1

B

Supplier	Substance	Batch	Spectra
Caelo	Barberries	11058320	1
Caelo	Barberries	12217103	3
Caelo	Barberries	12217106	1
Caelo	Barberries	12217111	1
Caelo	Barberries	12217113	2
Caelo	Barberries	12217116	1
Caelo	Barberries	16224202	1
Caelo	Barberries	12217107	1
Caelo	Barberries	1221707	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Barberries	12217109	4
Caelo	Barberry root bark, cut	11083509	1
Caelo	Barberry root bark, cut	55B110128	1
Caelo	Barberry root bark, cut	12112606	5
Caelo	Barberry root bark, cut	12112603	2
Caelo	Barberry root bark, cut	12112605	1
Klenk	Barberry root bark, cut	551B110128	4
Klenk	Barberry root bark, cut	551B120320	1
Caelo	Barberry root bark, cut	12112608	1
Fagron	Barbital sodium	15L07-B02	1
Klenk	Basil, rubbed	3632A110201	3
Caelo	Basil, rubbed	12066404	1
Caelo	Basil, rubbed	12007010	4
Caelo	Basil, rubbed	12007008	2
Caelo	Basil, rubbed	13048601	2
Caelo	Basil, rubbed	13048605	1
Caelo	Basil, rubbed	13048605-3519411022	1
Klenk	Basil, rubbed	3632A120502	4
Klenk	Basil, rubbed	A110201	1
Klenk	Basil, rubbed	A120502	1
Klenk	Basil, rubbed	3632a120502	1
VDL	Basil, rubbed	12007004	1
Aurica/Phönix	Bean shells	5052301	1
Bombastus	Bean shells	272781	3
Bombastus	Bean shells	278686	1
Bombastus	Bean shells	282475	1
Bombastus	Bean shells	278696	2
Bombastus	Bean shells	270517	1
Bombastus	Bean shells	240503	1
Cae	Bean shells	Int.Ch.313011	1
Caelo	Bean shells	29091201	1
Caelo	Bean shells	8301004	1
Caelo	Bean shells	6031301	1
Caelo	Bean shells	11030604	6
Caelo	Bean shells	1103061	1
Caelo	Bean shells	11030601	1
Caelo	Bean shells	13333801	1
Caelo	Bean shells	1333802	1
Caelo	Bean shells	13333803	1
Caelo	Bean shells	14080002	1
Caelo	Bean shells	15060905	1
Caelo	Bean shells	12358703	5
Caelo	Bean shells	10006507	1
Caelo	Bean shells	11233603	1
Caelo	Bean shells	11030602	5
Caelo	Bean shells	11030605	1
Galke	Bean shells	21219	1
Klenk	Bean shells	671A100816	2
Klenk	Bean shells	171A110301	1
Klenk	Bean shells	C120321	2
Klenk	Bean shells	671C121105	8
Klenk	Bean shells	C121105	2
Klenk	Bean shells	671C130620	6
Klenk	Bean shells	C130620	1
Klenk	Bean shells	671A110420	9
Klenk	Bean shells	671B180726	1
Klenk	Bean shells	671A180925	1
Klenk	Bean shells	671A-110420	1
Klenk	Bean shells	671A110301	1
Klenk	Bean shells	671C120321	16

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Bearberry leaf	12186506	3
Bombastus	Bearberry leaf	272297	8
Bombastus	Bearberry leaf	275491	3
Bombastus	Bearberry leaf	267926	1
Caelo	Bearberry leaf	11213011	3
Caelo	Bearberry leaf	20111210	1
Caelo	Bearberry leaf	11213010	1
Caelo	Bearberry leaf	13067802	3
Caelo	Bearberry leaf	12186503	1
Caelo	Bearberry leaf	15051303	1
Caelo	Bearberry leaf	4091301	1
Caelo	Bearberry leaf	13067805	6
Caelo	Bearberry leaf	5111301	1
Caelo	Bearberry leaf	12186504	1
Caelo	Bearberry leaf	17121306	1
Caelo	Bearberry leaf	4021407	1
Caelo	Bearberry leaf	15116201	1
Caelo	Bearberry leaf	17311305	1
Caelo	Bearberry leaf	17311308	1
Caelo	Bearberry leaf	1218602	1
Caelo	Bearberry leaf	280889	3
Caelo	Bearberry leaf	11213005	4
Caelo	Bearberry leaf	412A-01518	1
Caelo	Bearberry leaf	18304202	2
Caelo	Bearberry leaf	13067805-3390311080	1
Klenk	Bearberry leaf	2391b120314	2
Galke	Bearberry leaf	19936	3
Klenk	Bearberry leaf	2391B120314	6
Klenk	Bearberry leaf	2391B130328	9
Klenk	Bearberry leaf	2391B07030901	1
Caelo	Bearberry leaf	12186502	1
Sanacorp	Bearberry leaf	2391B110209	3
Klenk	Bearberry leaf	2391B120719	13
Caelo	Bentonite	fürHerrSalloch	1
Caelo	Bentonite	1307016-01	1
Caelo	Bentonite	1311014-01	1
Clariant - Mindel-Food	Bentonite	1301	1
Noweda	Bentonite	11304415	1
Euro OTC	Betaine hydrochloride	1202008-01	1
Euro OTC	Betaine hydrochloride	L1701040-01	1
Euro OTC	Betaine hydrochloride	1305027-01	2
Euro OTC	Betaine hydrochloride	L1510011-03	1
Euro OTC	Betaine hydrochloride	1510011-02	1
Euro OTC	Betaine hydrochloride	L1412019-01	1
Fagron	Betaine hydrochloride	12C20-N09	1
Fagron	Betaine hydrochloride	24091301	1
Fagron	Betaine hydrochloride	15121401	1
Gatt-Koller	Betaine hydrochloride	2970/07102910	1
Fagron	Betaine hydrochloride	13G29-B02-294870	1
Bombastus	Betony herb, cut	12007205	2
Caelo	Betony herb, cut	12007208	1
Caelo	Betony herb, cut	13048906	1
Caelo	Betony herb, cut	134048903	1
Caelo	Betony herb, cut	13367802	1
Sanacorp	Betony herb, cut	13048903	3
Caelo	Betony herb, cut	12007201	1
Anzag	Bilberry fruit, dried	2910N120921	2
Cae	Bilberry fruit, dried	212172	1
Caelo	Bilberry fruit, dried	13130504	1
Caelo	Bilberry fruit, dried	12183701	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Bilberry fruit, dried	26061301	1
Caelo	Bilberry fruit, dried	10265601	1
Caelo	Bilberry fruit, dried	18101307	1
Caelo	Bilberry fruit, dried	13130501	1
Caelo	Bilberry fruit, dried	10273708	1
Caelo	Bilberry fruit, dried	10273709	1
Caelo	Bilberry fruit, dried	10265603	1
Caelo	Bilberry fruit, dried	10273711	1
Caelo	Bilberry fruit, dried	12183704	4
Fiebig 05.11.12 ek...	Bilberry fruit, dried	2910A120410	1
Klenk	Bilberry fruit, dried	2910N110304	5
Klenk	Bilberry fruit, dried	2010N110304	1
Klenk	Bilberry fruit, dried	2910A090717	1
Klenk	Bilberry fruit, dried	2910N130131	11
Klenk	Bilberry fruit, dried	N130131	2
Klenk	Bilberry fruit, dried	N121022	1
Klenk	Bilberry fruit, dried	2910n130131	1
Klenk	Bilberry fruit, dried	910N130131	1
Klenk	Bilberry fruit, dried	2910n110304	1
Klenk	Bilberry fruit, dried	2910N121022	7
Bombastus	Bilberry leaf	272176	2
Caelo	Bilberry leaf	13009904	3
Caelo	Bilberry leaf	9367603	2
Caelo	Bilberry leaf	23111201	1
Caelo	Bilberry leaf	12140206	2
Caelo	Bilberry leaf	3091302	1
Caelo	Bilberry leaf	13009907	2
Caelo	Bilberry leaf	12140201	2
Caelo	Bilberry leaf	13009901	3
Caelo	Bilberry leaf	13009903	4
Caelo	Bilberry leaf	1300907	1
Klenk	Bilberry leaf	4042013	1
Klenk	Bilberry leaf	2191N110516	5
Klenk	Bilberry leaf	N110516	1
Sanacorp	Bilberry leaf	2191A130410	2
Caelo	Bilberry leaf	12140204	4
Aurica	Birch leaf	521205644	1
Bahnhof-Apotheke	Birch leaf	18-120702	1
Bombastus	Birch leaf	280677	1
Bombastus	Birch leaf	287280	1
Bombastus	Birch leaf	272385	1
Bombastus	Birch leaf	267077	1
Bombastus	Birch leaf	270743	1
Caelo	Birch leaf	11189510	3
Caelo	Birch leaf	11189507	1
Caelo	Birch leaf	11189508	1
Caelo	Birch leaf	12193109	15
Caelo	Birch leaf	IntCh:311092	1
Caelo	Birch leaf	12193108	1
Caelo	Birch leaf	13108906	1
Caelo	Birch leaf	13337303	1
Caelo	Birch leaf	13337302	1
Caelo	Birch leaf	13108917	1
Caelo	Birch leaf	14360702	1
Caelo	Birch leaf	13108916	1
Caelo	Birch leaf	12193104	1
Caelo	Birch leaf	107063	1
Caelo	Birch leaf	11189502	1
Caelo	Birch leaf	12193004	5
Caelo	Birch leaf	12193105	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Birch leaf	13337303-3561412013	1
Caesar & Loretz Gm…	Birch leaf	11050102	3
Fagron	Birch leaf	7061301	1
Galke	Birch leaf	20904	1
Galke	Birch leaf	21226	1
Klenk	Birch leaf	1901A110726	24
Klenk	Birch leaf	1901c120508	1
Klenk	Birch leaf	20111201	1
Klenk	Birch leaf	1901C120508	18
Klenk	Birch leaf	F-040413-1	1
Klenk	Birch leaf	C120802	1
Klenk	Birch leaf	21061303	1
Klenk	Birch leaf	A121130	2
Klenk	Birch leaf	1901A121130	24
Klenk	Birch leaf	1901c120802	1
Klenk	Birch leaf	28101306	1
Klenk	Birch leaf	27121301	1
Klenk	Birch leaf	1901A130218	5
Klenk	Birch leaf	4021409	1
Klenk	Birch leaf	1901A130318	2
Klenk	Birch leaf	1901A140214	1
Klenk	Birch leaf	1901A-110726	3
Klenk	Birch leaf	1901C120802	19
Klenk	Birch leaf	4213I01481	1
Klenk	Birch leaf	1901A05051801	1
Klenk	Birch leaf	4113A-01481	1
Caelo	Birch leaf	13108905	8
Spangropharm	Birch leaf	264603	1
5N Plus Lübeck Gmb…	Bismuth subnitrate, heavy	12146908	1
Caelo	Bismuth subnitrate, heavy	12146903	4
Caelo	Bismuth subnitrate, heavy	12146902	1
Caelo	Bismuth subnitrate, heavy	12146911	3
Caelo	Bismuth subnitrate, heavy	4513M-01186	1
Caelo	Bismuth subnitrate, heavy	12146913	2
Caelo	Bismuth subnitrate, heavy	M468105	1
Caelo	Bismuth subnitrate, heavy	10013208	1
Caelo	Bismuth subnitrate, heavy	10F09-N13	1
Caelo	Bismuth subnitrate, heavy	10013213	1
Caelo	Bismuth subnitrate, heavy	11052805	1
Caelo	Bismuth subnitrate, heavy	11052809	1
Caesar & Loretz/ Noweda	Bismuth subnitrate, heavy	12145701	1
Fagron	Bismuth subnitrate, heavy	1309211186	1
Fagron	Bismuth subnitrate, heavy	12C08-N06	3
Fagron	Bismuth subnitrate, heavy	12D26-N03	1
Fagron	Bismuth subnitrate, heavy	1001311186	1
Fagron	Bismuth subnitrate, heavy	13C15-N05	3
Fagron	Bismuth subnitrate, heavy	13H28-B04-291385	1
Fagron	Bismuth subnitrate, heavy	11D28-N16	1
Fagron	Bismuth subnitrate, heavy	13B25-N02	3
Fagron	Bismuth subnitrate, heavy	11/13-N01	1
Merck	Bismuth subnitrate, heavy	75419201	1
Noweda	Bismuth subnitrate, heavy	13/01-N02	1
Purren Apotheke	Bismuth subnitrate, heavy	11H31-N06	1
Sanacorp	Bismuth subnitrate, heavy	12146909	2
-	Bitter-Orange flower (petals)	2011A-01445	1
Caelo	Bitter-Orange flower (petals)	11049212	1
Caelo	Bitter-Orange flower (petals)	12266703	2
Caelo	Bitter-Orange flower (petals)	11049202	1
Caelo	Bitter-Orange flower (petals)	12266608	6

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Bitter-Orange flower (petals)	2712E-01445	1
Caelo	Bitter-Orange flower (petals)	12266609	1
Caelo	Bitter-Orange flower (petals)	6051301	1
Caelo	Bitter-Orange flower (petals)	12266708	1
Caelo	Bitter-Orange flower (petals)	13067903	2
Caelo	Bitter-Orange flower (petals)	12266705	1
Caelo	Bitter-Orange flower (petals)	12266614	1
Caelo	Bitter-Orange flower (petals)	13352701	1
Caelo	Bitter-Orange flower (petals)	12266707	1
Caelo	Bitter-Orange flower (petals)	12266605	1
Caelo	Bitter-Orange flower (petals)	12266611	1
Caelo	Bitter-Orange flower (petals)	12266608	2
Caelo	Bitter-Orange flower (petals)	12266605	1
Caelo	Bitter-Orange flower (petals)	12266611	1
Caelo	Bitter-Orange flower (petals)	13352701-3518411022	1
Hepart AG	Bitter-Orange flower (petals)	B120822	1
Klenk	Bitter-Orange flower (petals)	1201B120822	1
Klenk	Bitter-Orange flower (petals)	1201B110809	1
Klenk	Bitter-Orange flower (petals)	3613m-01445	1
Bombastus	Bitter-Orange peel	278233	4
Bombastus	Bitter-Orange peel	274240	3
Caelo	Bitter-Orange peel	12239203	3
Caelo	Bitter-Orange peel	12067402	1
Caelo	Bitter-Orange peel	17111201	1
Caelo	Bitter-Orange peel	12067405	1
Caelo	Bitter-Orange peel	4312M-01531	1
Caelo	Bitter-Orange peel	13049001	1
Caelo	Bitter-Orange peel	21101302	1
Caelo	Bitter-Orange peel	27011403	1
Klenk	Bitter-Orange peel	511B110321	2
Klenk	Bitter-Orange peel	2711B111207	1
Klenk	Bitter-Orange peel	511B120830	4
Klenk	Bitter-Orange peel	511A110411	1
Klenk	Bitter-Orange peel	B120830	1
Klenk	Bitter-Orange peel	C130226	3
Klenk	Bitter-Orange peel	511C130226	1
Klenk	Bitter-Orange peel	3613M-01531	1
kräuter schulte	Bitter-Orange peel	51265	1
Caelo	Black cohosh	10281112	1
Caelo	Black cohosh	10281104	1
Caelo	Black cohosh	10281118	2
Caelo	Black cohosh	13142101	1
Caelo	Black cohosh	13237907	1
Caelo	Black cohosh	51981386	1
Caelo	Black cohosh	13237903	1
Klenk	Black cohosh	6721B141202	1
Caelo	Black cohosh	13237901	2
Klenk	Black cohosh	6721B130214	10
Klenk	Black cohosh	B130528	2
Klenk	Black cohosh	6721B1130528	1
Klenk	Black cohosh	3794377	1
Klenk	Black cohosh	6721B081208	1
Klenk	Black cohosh	6721b130528	1
Kräuter Schulte	Black cohosh	3308M-02176	1
Nachprüfung	Black cohosh	10281113	1
Klenk	Black cohosh	6721B130528	3
Akazie	Black cumin seed	20.09.2015	1
Caelo	Black cumin seed	10121916	1
Caelo	Black cumin seed	10121915	1
Caelo	Black cumin seed	11233502	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Black cumin seed	12358901	2
Caelo	Black cumin seed	12358906	2
Caelo	Black cumin seed	13326405	2
Caelo	Black cumin seed	13326406	1
Caelo	Black cumin seed	14359903	3
Caelo	Black cumin seed	14359905	1
Caelo	Black cumin seed	16115710	1
Caelo	Black cumin seed	12358903	2
Caelo	Black cumin seed	16115708	3
Caelo	Black cumin seed	15300401	3
Caelo	Black cumin seed	16115706	1
Caelo	Black cumin seed	11233507	1
Caelo	Black cumin seed	13122013b	1
Caelo	Black cumin seed	16115703	2
Chiesi/Phönix	Black cumin seed	14359906	2
Hepart AG	Black cumin seed	20720,kbA	1
Caelo	Black cumin seed	12358902	1
Caelo	Black cumin seed	12358904	1
Klenk	Black cumin seed	7330A120703	1
Klenk	Black cumin seed	A120703	1
Caelo	Black cumin seed	11233503	1
Spinnrad	Black cumin seed	11931059	1
Spinnrad/Phoenix	Black cumin seed	613310592	1
Wolf	Black cumin seed		1
Wolf	Black cumin seed	20720	8
Wolf	Black cumin seed	B-471	1
Wolf	Black cumin seed	207204	1
Wolf	Black cumin seed	L310F141b	6
Wolf	Black cumin seed	L402F1713	1
Wolf	Black cumin seed	L402F171b	3
Caelo	Black mustard seed	12189307	1
Caelo	Black mustard seed	14057702	1
Caelo	Black mustard seed	16139102	1
Caelo	Black mustard seed	13038904	1
Klenk	Black mustard seed	7430A120813	2
Caelo	Black mustard seed, powdered	17196303	4
Klenk	Black mustard seed, powdered	7434A120712	1
Caelo	Black mustard seed, powdered	16051810	4
Caelo	Black mustard seed, powdered	12009702	4
Caelo	Black mustard seed, powdered	12009706	1
Caelo	Black mustard seed, powdered	12208602	5
Caelo	Black mustard seed, powdered	12208601	3
Caelo	Black mustard seed, powdered	12350202	16
Caelo	Black mustard seed, powdered	12350205	2
Caelo	Black mustard seed, powdered	12350208	7
Caelo	Black mustard seed, powdered	12350204	2
Caelo	Black mustard seed, powdered	12350210	1
Caelo	Black mustard seed, powdered	12350211	3
Caelo	Black mustard seed, powdered	13097705	6
Caelo	Black mustard seed, powdered	12350209	1
Caelo	Black mustard seed, powdered	13097704	4
Caelo	Black mustard seed, powdered	13358302	13
Caelo	Black mustard seed, powdered	25011401	1
Caelo	Black mustard seed, powdered	13358304	4
Caelo	Black mustard seed, powdered	23061401	1
Caelo	Black mustard seed, powdered	14162810	2
Caelo	Black mustard seed, powdered	14293702	6
Caelo	Black mustard seed, powdered	14162802	1
Caelo	Black mustard seed, powdered	15131102	3
Caelo	Black mustard seed, powdered	15214703	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Black mustard seed, powdered	15214707	1
Caelo	Black mustard seed, powdered	15214713	2
Caelo	Black mustard seed, powdered	16051807	1
Caelo	Black mustard seed, powdered	12208604	3
Caelo	Black mustard seed, powdered	11276701	1
Caelo	Black mustard seed, powdered	12009703	1
Caelo	Black mustard seed, powdered	15214714	1
Caelo	Black mustard seed, powdered	16051807	1
Caelo	Black mustard seed, powdered	15131101	1
Caelo	Black mustard seed, powdered	16272704	2
Caelo	Black mustard seed, powdered	14293706	1
Caelo	Black mustard seed, powdered	15214707	2
Caelo	Black mustard seed, powdered	13097701	11
Caelo	Black mustard seed, powdered	13097702	4
Caelo	Black mustard seed, powdered	2015Q-02244	1
Caelo	Black mustard seed, powdered	17196306	1
Caelo	Black mustard seed, powdered	14162807	3
Caelo	Black mustard seed, powdered	14162810	3
Caelo	Black mustard seed, powdered	14245601	1
Caelo	Black mustard seed, powdered	14293701	2
Caelo	Black mustard seed, powdered	14293710	2
Caelo	Black mustard seed, powdered	15131104	1
Caelo	Black mustard seed, powdered	15214703	7
Caelo	Black mustard seed, powdered	16272703	6
Caelo	Black mustard seed, powdered	16272707	4
Caelo	Black mustard seed, powdered	16333501	2
Caelo	Black mustard seed, powdered	1633503	1
Caelo	Black mustard seed, powdered	17196301	1
Caelo	Black mustard seed, powdered	15131105	1
Caelo	Black mustard seed, powdered	15214706	3
Caelo	Black mustard seed, powdered	14162808	1
Caelo	Black mustard seed, powdered	14293713	1
Caelo	Black mustard seed, powdered	15214708	4
Caelo	Black mustard seed, powdered	12350202-3369319012	1
Caelo	Black mustard seed, powdered	13097706	2
Caelo	Black mustard seed, powdered	12350207	5
Caesar / Ebert & Jacobi	Black mustard seed, powdered	16051809	1
Caesar/ Noweda	Black mustard seed, powdered	14293711	3
Caelo	Black mustard seed, powdered	16333503	3
Caelo	Black mustard seed, powdered	17276404	1
Klenk	Black mustard seed, powdered	A130422	1
Klenk	Black mustard seed, powdered	7434A130422	3
Klenk	Black mustard seed, powdered	7434A140923	2
Klenk	Black mustard seed, powdered	7434A150608	4
Klenk	Black mustard seed, powdered	7434a150608	1
Noweda/Henry Lamotte	Black mustard seed, powdered	1493708	1
Caelo	Black mustard seed, powdered	16051802	3
Anzag	Blackberry leaf	10136412	1
Anzag 27.12.12 ek:2,79	Blackberry leaf	10136048	1
Bahnhof-Apotheke	Blackberry leaf	18-120702	1
Bombastus	Blackberry leaf	267122	1
Bombastus	Blackberry leaf	273668	2
Caelo	Blackberry leaf	2271c120508	1
Caelo	Blackberry leaf	10136403	1
Caelo	Blackberry leaf	10136408	6
Caelo	Blackberry leaf	28061202	1
Caelo	Blackberry leaf	13091206	1
Caelo	Blackberry leaf	11030704	4
Caelo	Blackberry leaf	11030707	5
Caelo	Blackberry leaf	3011E-01512	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Blackberry leaf	11030706	1
Caelo	Blackberry leaf	3091303	1
Caelo	Blackberry leaf	14111318	1
Caelo	Blackberry leaf	13127901	1
Caelo	Blackberry leaf	13101610	1
Caelo	Blackberry leaf	14019010	1
Caelo	Blackberry leaf	15039301	1
Caelo	Blackberry leaf	11030701	2
Gehe	Blackberry leaf	10136409	1
Klenk	Blackberry leaf	2271B111216	1
Caelo	Blackcurrant leaf, cut	9373913	1
Caelo	Blackcurrant leaf, cut	12115902	1
Caelo	Blackcurrant leaf, cut	12168804	1
Caelo	Blackcurrant leaf, cut	12168810	3
Caelo	Blackcurrant leaf, cut	80558228	1
Klenk	Blackcurrant leaf, cut	2251a110204	1
Nachprüfung	Blackcurrant leaf, cut	1003	1
Sanacorp	Blackcurrant leaf, cut	2251A110204	4
Caelo	Blackcurrants	12272804	3
Caelo	Blackcurrants	14212507	1
Galke	Blackcurrants	21348	1
Klenk	Blackcurrants	A121106	1
Klenk	Blackcurrants	2990A110620	1
Caelo	Blackthorn flower	12178101	2
Caelo	Blackthorn flower	11206906	1
Caelo	Blackthorn flower	12178104	4
Caelo	Blackthorn flower	12178105	1
Caelo	Blackthorn flower	12178102	9
Caelo	Blackthorn flower	12178103	2
Klenk	Blackthorn flower	2612E-01468	1
Caelo	Blackthorn flower, rubbed	1150N101109	2
Klenk	Blackthorn flower, rubbed	N101109	2
Klenk	Blackthorn flower, rubbed	1150n101109	1
Kräuter Schulte	Blackthorn flower, rubbed	53233	2
an	Blessed thistle, cut	13389704	1
Anzag	Blessed thistle, cut	282281	1
Bombastus	Blessed thistle, cut	271946	1
Caelo	Blessed thistle, cut	9355208	1
Caelo	Blessed thistle, cut	27111205	1
Caelo	Blessed thistle, cut	10325402	5
Caelo	Blessed thistle, cut	4743554	1
Caelo	Blessed thistle, cut	13025901	5
Caelo	Blessed thistle, cut	13025902	1
Caelo	Blessed thistle, cut	12038202	1
Caelo	Blessed thistle, cut	3091301	1
Caelo	Blessed thistle, cut	13025903	3
Caelo	Blessed thistle, cut	12038203	2
Caelo	Blessed thistle, cut	10325404	1
Caelo	Blessed thistle, cut	13389701	1
Gehe / 08.03.13 Redwood	Blessed thistle, cut	205007	1
Klenk	Blessed thistle, cut	A110517	1
Apofit	Blue bottle flower	278776	1
Bombastus	Blue bottle flower	275759	2
Bombastus	Blue bottle flower	284030	1
Caelo	Blue bottle flower	11059209	2
Caelo	Blue bottle flower	12060203	4
Caelo	Blue bottle flower	12232501	2
Caelo	Blue bottle flower	12060202	2
Caelo	Blue bottle flower	14323302	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Blue bottle flower	15206601	1
Caelo	Blue bottle flower	72767368	1
Caelo	Blue bottle flower	12060205	4
Caelo	Blue bottle flower	11059206	2
Caelo	Blue bottle flower	11059211	2
Galke	Blue bottle flower	23131	2
Klenk	Blue bottle flower		1
Caelo	Bogbean leaf, cut	12226101	1
Caelo	Bogbean leaf, cut	1226101	1
Caelo	Bogbean leaf, cut	13123901	2
Caelo	Bogbean leaf, cut	13123902	2
Caelo	Bogbean leaf, cut	12226104	1
Caesar/Noweda	Bogbean leaf, cut	1510U-01517	1
Caelo	Bogbean leaf, cut	13149001	1
Caelo	Boldo leaf	11016509	1
Caelo	Boldo leaf	655456	1
Caelo	Boldo leaf	11016511	1
Caelo	Boldo leaf	12064303	1
Caelo	Boldo leaf	12227005	1
Caelo	Boldo leaf	12064305	1
Caelo	Boldo leaf	12064306	1
Caelo	Boldo leaf	12227004	1
Galke	Boldo leaf	19855	1
Klenk	Boldo leaf	1911B090709	1
Klenk	Boldo leaf	1911A100714	7
VDL	Boldo leaf	11016503	1
Caelo	Bucho leaf	13056601	2
Caelo	Bucho leaf	13056602	2
Caelo	Bucho leaf	13056605	1
Kräuter Schulte	Bucho leaf	54519	1
Caelo	Buckwheat herb, cut	11212612	1
Caelo	Buckwheat herb, cut	11212808	2
Caelo	Buckwheat herb, cut	30041301	1
Caelo	Buckwheat herb, cut	2051303	1
Caelo	Buckwheat herb, cut	13051303	1
Caelo	Buckwheat herb, cut	11212809	1
Caelo	Buckwheat herb, cut	11212817	6
Caelo	Buckwheat herb, cut	11212807	2
Caelo	Buckwheat herb, cut	5111302	1
Caelo	Buckwheat herb, cut	11212810	1
Caelo	Buckwheat herb, cut	11212814	2
Caelo	Buckwheat herb, cut	13193203	1
Hepart AG	Buckwheat herb, cut	B120509	2
Klenk	Buckwheat herb, cut	4581B120509	3
Caelo	Buckwheat herb, cut	11212812	1
-	Burdock root	5110I-02131	1
Caelo	Burdock root	12295808	2
Caelo	Burdock root	12295801	2
Caelo	Burdock root	1100801	1
Caelo	Burdock root	10073213	1
Caelo	Burdock root	11100801	2
Caelo	Burdock root	12295805	3
Caelo	Burdock root	12295807	1
Caelo	Burdock root	13122802	1
Caelo	Burdock root	13122801	2
Caelo	Burdock root	12295802	4
Caelo	Burdock root	107063	1
Euro OTC	Burdock root	13122803	1
Galke	Burdock root	19802	1
Klenk	Burdock root	6161A101206	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Burdock root	6161A120208	4
Klenk	Burdock root	A120206	1
Klenk	Burdock root	A130214	1
Klenk	Burdock root	6161A080709	1
Klenk	Burdock root	6161A-101206	1
Klenk	Burdock root	6161A120103	1
Klenk	Burdock root	6161A-120103	1
Caelo	Burnet root	8111203	1
Caelo	Burnet root	12027411	3
Caelo	Burnet root	12027405	2
Caelo	Burnet root	12027403	1
Caelo	Burnet root	12027413	1
Caelo	Burnet root	12027409	1
Caelo	Burnet root	12027410	3

C

Supplier	Substance	Batch	Spectra
Caelo	Calcium chloride dihydrate	12341409	1
Caelo	Calcium chloride dihydrate	11230921	2
Caelo	Calcium chloride dihydrate	12341404	2
Caelo	Calcium chloride dihydrate	11230915	1
Caelo	Calcium chloride dihydrate	12341406	1
Caelo	Calcium chloride dihydrate	12B09-N11	1
EUro/AHD	Calcium chloride dihydrate	1205014-02	2
Caelo	Calcium chloride dihydrate	8237314	1
Fagron	Calcium hydroxide	12J18-N01	1
Fagron	Calcium hydroxide	13D26-N14	1
Gehe	Calcium hydroxide	12F08-N02	3
Euro OTC	Calcium orotate dihydrate	1401006-01	1
Euro OTC	Calcium orotate dihydrate	1203037-01	2
Caelo	Calcium sulfate dihydrate	10132403	1
Caelo	Calcium sulfate dihydrate	12316301	1
Caelo	Calcium sulfate hemihydrate	14101701	1
Caelo	Calcium sulfate hemihydrate	9246320	1
Bombastus	Calendula flower	268626	1
Caelo	Calendula flower	12221706	2
Caelo	Calendula flower	13235503	3
Caelo	Calendula flower	15291501	1
Caelo	Calendula flower	12221710	1
Caelo	Calendula flower	12221705	1
Caelo	Calendula flower	12221511	1
Caelo	Calendula flower	12221508	1
Caelo	Calendula flower	122221707	1
Caelo	Calendula flower	12221708	3
Caelo	Calendula flower	12221510-3356319071	1
Caelo	Calendula flower	12221510-3435311151	1
Caelo	Calendula flower	13235502	3
galke,	Calendula flower	12028	1
Bombastus	Calendula flower	280306	1
Klenk	Calendula flower	1250A110511	1
Klenk	Calendula flower	C120321	1
Klenk	Calendula flower	1241B120312	1
Klenk	Calendula flower	1241B130517	1
Wolf	Calendula flower	23342	1
Anzag	Calendula flower, cut	12221706	12
Bahnhof-Apotheke	Calendula flower, cut	17-121106	1
Bombastus	Calendula flower, cut	270046	1
Bombastus	Calendula flower, cut	253620	1
Bombastus	Calendula flower, cut	279632	1
Bombastus	Calendula flower, cut	275813	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Calendula flower, cut	275128	1
Bombastus	Calendula flower, cut	207294	1
Bombastus	Calendula flower, cut	234997	1
Caelo	Calendula flower, cut	13235502	9
Caelo	Calendula flower, cut	295556	1
Caelo	Calendula flower, cut	22061203	1
Caelo	Calendula flower, cut	12071201	1
Caelo	Calendula flower, cut	11187612	12
Caelo	Calendula flower, cut	11187610	3
Caelo	Calendula flower, cut	27101201	1
Caelo	Calendula flower, cut	19111206	1
Caelo	Calendula flower, cut	11187611	3
Caelo	Calendula flower, cut	31121202	1
Caelo	Calendula flower, cut	5021305	1
Caelo	Calendula flower, cut	12221705	4
Caelo	Calendula flower, cut	11221407	1
Caelo	Calendula flower, cut	12221704	13
Caelo	Calendula flower, cut	8041302	1
Caelo	Calendula flower, cut	3061301	1
Caelo	Calendula flower, cut	12221707	2
Caelo	Calendula flower, cut	21091301	1
Caelo	Calendula flower, cut	12221710	2
Caelo	Calendula flower, cut	9112013C	1
Caelo	Calendula flower, cut	13235501	4
Caelo	Calendula flower, cut	9121303	1
Caelo	Calendula flower, cut	18121301	1
Caelo	Calendula flower, cut	13235505	1
Caelo	Calendula flower, cut	13410202	2
Caelo	Calendula flower, cut	15040301	1
Caelo	Calendula flower, cut	10291904	1
Caelo	Calendula flower, cut	12221701	1
Caelo	Calendula flower, cut	122221704	1
Caelo	Calendula flower, cut	1187612	2
Caelo	Calendula flower, cut	12221708	11
Caelo	Calendula flower, cut	13235506	2
Caelo	Calendula flower, cut	AKD1	1
Caelo	Calendula flower, cut	1325502	1
Gehe	Calendula flower, cut	260205	1
Klenk	Calendula flower, cut	1241B130517	6
Klenk	Calendula flower, cut	1241B150902	1
Klenk	Calendula flower, cut	1241N151209	1
Klenk	Calendula flower, cut	1241B160530	1
Klenk	Calendula flower, cut	1241B120419	2
Klenk	Calendula flower, cut	112211448	1
Klenk	Calendula flower, cut	1240A110418	1
Klenk	Calendula flower, cut	204311448	1
Klenk	Calendula flower, cut	1241B130321	5
Klenk	Calendula flower, cut	3013E1448	1
Klenk	Calendula flower, cut	B130517	2
Klenk	Calendula flower, cut	1241B140211	1
Klenk	Calendula flower, cut	1241B130927	1
Klenk	Calendula flower, cut	1241B110118	2
Noweda	Calendula flower, cut	12221709	9
Klenk	Calendula flower, cut	1241C120321	4
Fagron	Calendula flower, cut	1241B120312	4
Sanacorp	Calendula flower, cut	12221601	4
Caelo	Calendula flower, cut	12221502	2
AHD	Camphor	17288306	18
Euro OTC	Camphor	1210030-02	1
an	Camphor	12344909	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Camphor	13205502	1
Caelo	Camphor	13195316	6
Caelo	Camphor		1
Caelo	Camphor	11286905	2
Caelo	Camphor	3091203	1
Caelo	Camphor	11032023	1
Caelo	Camphor	11074509	1
Caelo	Camphor	12054107	4
Caelo	Camphor	120564113	1
Caelo	Camphor	12054141	3
Caelo	Camphor	12344905	2
Caelo	Camphor	12054142	6
Caelo	Camphor	11286910	1
Caelo	Camphor	4101303	1
Caelo	Camphor	12054114	2
Caelo	Camphor	12243701	1
Caelo	Camphor	13205512	2
Caelo	Camphor	13205511	1
Caelo	Camphor	13195311	1
Caelo	Camphor	25041401	1
Caelo	Camphor	13195314	5
Caelo	Camphor	12061411	1
Caelo	Camphor	13195316	1
Caelo	Camphor	13205522	1
Caelo	Camphor	13205522	3
Caelo	Camphor	13195318	1
Caelo	Camphor	13K28-04-294937	1
Caelo	Camphor	13195322	7
Caelo	Camphor	4031503	1
Caelo	Camphor	13195327	1
Caelo	Camphor	13195326	3
Caelo	Camphor	14202807	3
Caelo	Camphor	15097803	2
Caelo	Camphor	15120901	2
Caelo	Camphor	14310705	1
Caelo	Camphor	15316807	7
Caelo	Camphor	15320604	5
Caelo	Camphor	1410710	1
Caelo	Camphor	14310713	11
Caelo	Camphor	15316819	7
Caelo	Camphor	150622C	1
Caelo	Camphor	140918C	1
Caelo	Camphor	1531611	1
Caelo	Camphor	15120902	1
Caelo	Camphor	16209304	3
Caelo	Camphor	14310710	2
Caelo	Camphor	14310718	6
Caelo	Camphor	15384201	1
Caelo	Camphor	15397701	1
Caelo	Camphor	16209305	11
Caelo	Camphor	16235405	2
Caelo	Camphor	14310722	3
Caelo	Camphor	16235404	4
Caelo	Camphor	16209306	1
Caelo	Camphor	15/18.B11-321658	1
Caelo	Camphor	162093029	1
Caelo	Camphor	17004304	1
Caelo	Camphor	17004302	4
Caelo	Camphor	17050605	30
Caelo	Camphor	13111707	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Camphor	13111708	1
Caelo	Camphor	1531607	1
Caelo	Camphor	17134703	4
Caelo	Camphor	17288301	11
Caelo	Camphor	17324104	10
Caelo	Camphor	7061802	1
Caelo	Camphor	7071801	1
Caelo	Camphor	17288305	1
Caelo	Camphor	18066404	9
Caelo	Camphor	12091805	1
Caelo	Camphor	12091808	1
Caelo	Camphor	17325503	1
Caelo	Camphor	17325502	1
Caelo	Camphor	18019806	26
Caelo	Camphor	6021901	1
Caelo	Camphor	18019807	2
Caelo	Camphor	18196902	1
Caelo	Camphor	1728306	1
Caelo	Camphor	17288360	1
Caelo	Camphor	18196910	1
Caelo	Camphor	18327910	2
Caelo	Camphor	18196907	1
Caelo	Camphor	192762009	2
Caelo	Camphor	20003828001	1
Caelo	Camphor	20004261002	1
Caelo	Camphor	15086806	1
Caelo	Camphor	16209301	12
Caelo	Camphor	1536801	1
Caelo	Camphor	13195301	1
Caelo	Camphor	13195301	2
Caelo	Camphor	13195304	1
Caelo	Camphor	13195311	1
Caelo	Camphor	16209309	24
Caelo	Camphor	12054149	9
Caelo	Camphor	444A170221	1
Caelo	Camphor	13195318	1
Caelo	Camphor	18327903P-191111-3	1
Caelo	Camphor	18019803P-190506-3	1
Caelo	Camphor	12228206	1
Caelo	Camphor	62(17288306)	1
Caelo	Camphor	3273	1
Caelo	Camphor	14310706	1
Caelo	Camphor	17050606	5
Caelo	Camphor	12054151	2
Caelo	Camphor	13195323	1
Caelo	Camphor	15316805	1
Caelo	Camphor	18108904	11
Caelo	Camphor	14224304	1
Caelo	Camphor	11286909	2
Caelo	Camphor	2344905	1
Caelo	Camphor	713A-01221	1
Caelo	Camphor	914E-01221	1
Caelo	Camphor	315E-01221	1
Caelo	Camphor	5315I-01221	1
Caelo	Camphor	218U-01221	1
Caelo	Camphor	14310715	1
Caelo	Camphor	14224303	3
Caelo	Camphor	1412023-01	7
Caelo	Camphor	18198003	1
Caelo	Camphor	18019603	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Camphor	18327905	3
Caelo	Camphor	18327909	2
Caelo	Camphor	12228205	1
Caelo	Camphor	12054124	2
Caelo	Camphor	12054143	1
Caelo	Camphor	2811Q-01221	1
Caelo	Camphor	13205512	1
Caelo	Camphor	15086801	1
Caelo	Camphor	15316806	2
Caelo	Camphor	15062701	1
Caelo	Camphor	15316815	4
Caelo	Camphor	16209310	1
Caelo	Camphor	17004307	1
Caelo	Camphor	13108106	2
Caelo	Camphor	13205501	2
Caelo	Camphor	19009704	5
Caelo	Camphor	17004308	2
Caelo	Camphor	14310705	14
Caelo	Camphor	14310703	1
Caelo	Camphor	13205511	2
Caelo	Camphor	2803020-01	1
Caelo	Camphor	14310709	6
Caelo	Camphor	4444A150721	1
Caelo	Camphor	13205517	1
Caelo	Camphor	14310109	1
Caelo	Camphor	15397704	5
Caelo	Camphor	15316823	3
Caelo	Camphor	17004301	21
Caelo	Camphor	18019803	14
Caelo	Camphor	12054105	1
Caelo	Camphor	13195314	3
Caelo	Camphor	13108118	2
Caelo	Camphor	14G23-B04-301879	2
Caelo	Camphor	15062702	3
Caelo	Camphor	15316801	4
Caelo	Camphor	15316812	1
Caelo	Camphor	16235407	1
Caelo	Camphor	16235402	1
Caelo	Camphor	2015113782	1
Caelo	Camphor	14310702	1
Caesar & Loretz GmbH	Camphor	18019811	15
Caesar & Loretz GmbH	Camphor	17288307	2
Caesar & Loretz GmbH	Camphor	18327901	2
Caesar & Loretz GmbH	Camphor	192762005	2
Caesar & Loretz Gm…	Camphor	11032035	4
Caesar & Loretz Gm…	Camphor	18019813	1
Caesar Loretz	Camphor	18327903	13
Caesar&Loretz	Camphor	14310719	1
Caesar/Noweda	Camphor	1032	1
Caesar/Noweda	Camphor	13195328	1
Calo/AHD	Camphor	15086803	1
Camphor & Allied P…	Camphor	16209302	1
Cealo/ Noweda	Camphor	13108116	1
EuRho	Camphor	2111E-01219	1
Euro OTC	Camphor	1210030-02	4
Euro OTC	Camphor	1202021	1
Euro OTC	Camphor	113Q-01221	1
Euro OTC	Camphor	121003001	1
Euro OTC	Camphor	130313-02	1
Euro OTC	Camphor	1309019-03	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Camphor	1210030-01	7
Euro OTC	Camphor	1101029-02/Ch241011	1
Euro OTC	Camphor	1210030-01	1
Euro OTC	Camphor	1406029-02	2
Euro OTC	Camphor	121003002	1
Euro OTC	Camphor	1202021-02	2
Euro OTC	Camphor	1406029-01	3
Euro OTC	Camphor	1101029-02	1
Euro OTC	Camphor	1303013-02	11
euro/ Sanacorp	Camphor	17050602	2
Euro OTC	Camphor	821509	1
Euro OTC	Camphor	1309019-02	1
Euro OTC	Camphor	2803020-01	1
Euro OTC	Camphor	1303013-01	5
Fagron	Camphor	12G02-N09	1
Fagron	Camphor	12D23-N03	1
Fagron	Camphor	11K23-N04	1
Fagron	Camphor	690442	1
Fagron	Camphor	13H23-B40-291888	1
Fagron	Camphor	13H23-B40-294116	1
Fagron	Camphor	8082014A	1
Fagron	Camphor	13h23-b40-294116	1
Fagron	Camphor	14G23-B04-296868	1
Fagron	Camphor	1309019-02	1
Fagron	Camphor	13K28-B04-289340	1
Fagron	Camphor	15/18-B11-321658	1
Fagron	Camphor	17L01-B03	1
Fagron	Camphor	13H23-B04-288376	1
Fagron	Camphor	13K28-B04-294937	1
Fagron	Camphor	14G23-B04-301878	3
Fagron	Camphor	14G23-B04-299202	2
Fagron	Camphor	27011	1
Fagron	Camphor	825653	1
Fagron	Camphor	14G23-B04	2
Fagron	Camphor	13K28-B04	1
Fagron	Camphor	13H23-B40-296252	1
Fagron	Camphor	11H30-N15	1
Fagron	Camphor	13K28-B04	2
Fagron	Camphor	13K28_B04_294933	1
Fagron	Camphor	15097801	1
Fagron	Camphor	12B14-N09	1
Galke	Camphor	23624	1
Gatt-Koller	Camphor	1800202	3
Gehe	Camphor	17134702	5
GEHE	Camphor	16235408	5
Caelo	Camphor	14224303	1
Caelo	Camphor	17050605/1140418	1
Klenk	Camphor	444A160817	8
Klenk	Camphor	444A150721	1
Klenk	Camphor	444A100826	1
Klenk	Camphor	444A180815	3
Klenk	Camphor	444A170224	4
Klenk	Camphor	444A150721	1
Klenk	Camphor	444A140526	5
L12	Camphor	18108901	1
Caelo	Camphor	15397705	1
Nachprüfung	Camphor	1616E-01221	1
Nachtestung-Verlän...	Camphor	242/17	1
Noweda	Camphor	1202021-01	3
Caelo	Camphor	14202801	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Phoenix	Camphor	15316811	8
Phoenix	Camphor	160209309	1
Phoenix	Camphor	3382	1
Caelo	Camphor	12054113	1
phönix	Camphor	444a160817	1
Phönix Gotha	Camphor	206/06	1
Caelo	Camphor	2018-05-07-AISe	1
Post-Apotheke 22.0...	Camphor	11032012	1
Sanacorp	Camphor	444A130115	1
Sanacorp	Camphor	14310720	2
Sanacorp	Camphor	17004306	11
Sanacorp	Camphor	18019802	9
Caelo	Camphor	15097802	2
Caelo	Camphor	18108902	1
Caelo	Camphor	18108905	2
Vögele	Camphor	2014101206	1
Vögele	Camphor	2016114336	1
xxx	Camphor	709E-01221	1
Alfred Galke	Caraway fruit	20069	1
Anzag ek: 2,59EUR 19...	Caraway fruit	11003216	3
Caelo	Caraway fruit	12226609	5
Bahnhof-Apotheke	Caraway fruit	18-120709	1
Bombastus	Caraway fruit	275849	1
Bombastus	Caraway fruit	282269	1
Bombastus	Caraway fruit	270124	1
Caelo	Caraway fruit	12226603	7
Caelo	Caraway fruit	12226606	2
Caelo	Caraway fruit	12226504	1
Caelo	Caraway fruit	11003207	1
Caelo	Caraway fruit	27121202	1
Caelo	Caraway fruit	12343403	1
Caelo	Caraway fruit	11003211	1
Caelo	Caraway fruit	2103311537	1
Caelo	Caraway fruit	12226601	1
Caelo	Caraway fruit	4061303	1
Caelo	Caraway fruit	11378309	1
Caelo	Caraway fruit	413M	1
Caelo	Caraway fruit	12226614	2
Caelo	Caraway fruit	1226608	1
Caelo	Caraway fruit	13306003	1
Caelo	Caraway fruit	13397102	2
Caelo	Caraway fruit	13397104	2
Caelo	Caraway fruit	13091401	1
Caelo	Caraway fruit	13306004	1
Caelo	Caraway fruit	13306005	2
Caelo	Caraway fruit	13306006	4
Caelo	Caraway fruit	13306008	2
Caelo	Caraway fruit	15097109	3
Caelo	Caraway fruit	15097110	1
Caelo	Caraway fruit	16308502	1
Caelo	Caraway fruit	16165308	1
Caelo	Caraway fruit	15409105	1
Caelo	Caraway fruit	13306001	1
Caelo	Caraway fruit	24659273	1
Caelo	Caraway fruit	11121704	1
Caelo	Caraway fruit	18121717	1
Caelo	Caraway fruit	16308504	1
Caelo	Caraway fruit	11003217	5
Caelo	Caraway fruit	15409102	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Caraway fruit	12226611	3
Caelo	Caraway fruit	13306007	4
Caelo	Caraway fruit	15097101	8
Caelo	Caraway fruit	16308506	2
Caelo	Caraway fruit	15097102	1
Caelo	Caraway fruit	1509101	1
Caelo	Caraway fruit	13397105	8
Caelo	Caraway fruit	15097103	5
Caelo	Caraway fruit	290416	1
Caelo	Caraway fruit	15097115	6
Caelo	Caraway fruit	15409101	1
Caelo	Caraway fruit	12226501	5
Caelo	Caraway fruit	9267815	1
Caelo	Caraway fruit	811E-01537	1
Caelo	Caraway fruit	15097002	1
Caelo	Caraway fruit	17256303	2
Caelo	Caraway fruit	15097111	3
Caelo	Caraway fruit	15097116	1
Caelo	Caraway fruit	15409104	3
Caelo	Caraway fruit	18303903	1
Caelo	Caraway fruit	13306002	5
Caelo	Caraway fruit	15097108	4
Caelo	Caraway fruit	15409103	3
Caelo	Caraway fruit	16308501	2
Caelo	Caraway fruit	17256304	1
Caelo	Caraway fruit	18009206	1
Caelo	Caraway fruit	12226612	8
Caelo	Caraway fruit	15097107	2
Caeol/Phönix	Caraway fruit	16308503	5
Caesar & Loretz Gm...	Caraway fruit	9267824	2
Caesar & Loretz Gm...	Caraway fruit	11003213	2
Caesar & Loretz/Noweda	Caraway fruit	15056601	1
Galke	Caraway fruit	21257	1
Galke	Caraway fruit	23627	1
Galke	Caraway fruit	27450	1
GALKE	Caraway fruit	30030	1
Klenk	Caraway fruit	2770A130910	1
Hepart AG	Caraway fruit	B-224,kbA	1
Caelo	Caraway fruit	12226608	4
Caelo	Caraway fruit	1222608	1
Klenk	Caraway fruit	2770A110601	9
Klenk	Caraway fruit	2770A110818	8
Klenk	Caraway fruit	1810A-01537	1
Klenk	Caraway fruit	A120905	3
Klenk	Caraway fruit	2770A130521	12
Klenk	Caraway fruit	2270A130521	1
Klenk	Caraway fruit	412091-1-P	1
Klenk	Caraway fruit	2770A131008	2
Klenk	Caraway fruit	2820A150713	1
Klenk	Caraway fruit	2770A120403	14
Klenk	Caraway fruit	2770a120905	2
Klenk	Caraway fruit	5213A1537	1
Klenk	Caraway fruit	2770A140708	6
Klenk	Caraway fruit	2770A160304	2
Noweda	Caraway fruit	12226503	7
Noweda	Caraway fruit	12226605	3
Noweda	Caraway fruit	299573	2
Caelo	Caraway fruit	13041903	1
Caelo	Caraway fruit	15097118	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Caraway fruit	2041017/16308501	1
sanacorp	Caraway fruit	2656259	1
Sanacorp	Caraway fruit	2770A120905	4
Sanacorp	Caraway fruit		2
Caelo	Caraway fruit	15097117	1
Caelo	Caraway fruit	12226604	5
Caelo	Caraway fruit	13041901	1
Wolf	Caraway fruit	B-224	1
Caelo	Caraway fruit, pounded	12116904	3
Caelo	Caraway fruit, pounded	13367101	1
Galke	Caraway fruit, pounded	18943	1
apomix	Carbachol	12330703	1
Caelo	Cardamom fruit	11309110	1
Caelo	Cardamom fruit	13260502-3537411072	1
Klenk	Cardamom fruit	2750A110810	2
Klenk	Cardamom fruit	A110810	3
Klenk	Cardamom fruit	A130807	1
Caelo	Cardamom fruit	13026003	1
Caelo	Cayenne pepper, powdered (spice)	13205106	1
Klenk	Celery fruit	7140A170210	1
Caelo	Celery root, cut	12319105	2
Caelo	Celery root, cut	12319107	1
Caelo	Celery root, cut	10270009	1
Caelo	Celery root, cut	10270012	1
Caelo	Celery root, cut	12319108	1
Klenk	Celery root, cut	6091A110110	1
Bombastus	Centaury	277598	3
Aurica/Phönix	Centaury	520702152	1
Caelo	Centaury	12268608	10
Caelo	Centaury	11097605	2
Caelo	Centaury	11097609	3
Caelo	Centaury	10104012	1
Caelo	Centaury	8021302	1
Caelo	Centaury	15224102	1
Caelo	Centaury	12268606	14
Caelo	Centaury	12379601	1
Caelo	Centaury	11097602	1
Caelo	Centaury	3711B120628	1
Caelo	Centaury	12268601	3
Caelo	Centaury	12268605	4
Caelo	Centaury	12268602	19
Caelo	Centaury	16240512	1
Caelo	Centaury	18029609	1
Finze	Centaury	11097610	1
Galke	Centaury	9721	1
Klenk	Centaury	3711B111216	1
Klenk	Centaury	B120628	1
Klenk	Centaury	3711B-111216	1
Phoenix	Centaury	11097612	9
Phönix	Centaury	11093612	2
Klenk	Ceylon cinnamon, finely powdered	614B160818	1
Klenk	Ceylon cinnamon, finely powdered	614B120411	2
Klenk	Ceylon cinnamon, finely powdered	611B100628	1
Klenk	Ceylon cinnamon, finely powdered	614B121010	2
Klenk	Ceylon cinnamon, finely powdered	614b121024	1
Klenk	Ceylon cinnamon, finely powdered	614a120411	1
Klenk	Ceylon cinnamon, finely powdered	615B130325	3
Klenk	Ceylon cinnamon, finely powdered	614B121024	4
Caelo	Ceylonese Cinnamon, powdere…	12242806	2
Caelo	Ceylonese Cinnamon, powdere…	12242815	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ceylonese Cinnamon, powdere…	12242818	1
Klenk	Ceylonese Cinnamon, powdere…	614B161128	1
-	Chickweed, cut	2011A-01686	1
Caelo	Chickweed, cut	13040501	1
Caelo	Chickweed, cut	13040503	1
Caelo	Chickweed, cut	13254403	2
Caelo	Chickweed, cut	13254401	1
Caelo	Chickweed, cut	4551B130902	1
Caelo	Chickweed, cut	14212411	1
Caelo	Chickweed, cut	16143603	1
Caelo	Chickweed, cut	13040502-3283310662	1
Caelo	Chickweed, cut	16143608	2
Caelo	Chickweed, cut	13040502	2
Caelo	Chickweed, cut	13254404	1
Caelo	Chickweed, cut	13040504	1
Klenk	Chickweed, cut	4551b110222	1
Klenk	Chickweed, cut	4551B090528	1
Phoenix	Chickweed, cut	18100704	1
Caelo	Chickweed, cut	14212405	1
-	Chicory herb	4411I-01634	1
Caelo	Chicory herb	12034302	1
Caelo	Chicory herb	12034303	3
Caelo	Chicory herb	12354302	3
Caelo	Chicory herb	14031315	1
Caelo	Chicory herb	12354304	1
Caelo	Chicory herb	12354306	1
Caelo	Chicory herb	12369102	3
Caelo	Chicory herb	12034301	2
Klenk	Chicory herb	3751A120123	2
Klenk	Chicory herb	A120123	2
Klenk	Chicory herb	3751A080902	1
Klenk	Chicory herb	3751A120307	7
Klenk	Chicory herb	3751a120307	1
Klenk	Chicory herb	3751c120614	1
Klenk	Chicory herb	3751A-100118	1
Klenk	Chicory herb	4510I-01634	1
Sanacorp	Chicory herb	12369101	6
Klenk	Chicory root	66221A101202	1
Caelo	Chicory root	6221A101202	4
Caelo	Chicory root	11374501	1
Caelo	Chicory root	11374504	3
Caelo	Chicory root	11374506	1
Caelo	Chicory root	6221As101202	1
Caelo	Chicory root	11081803	1
Caelo	Chicory root	11374510	2
Caelo	Chicory root	91338319	1
Klenk	Chicory root	6221A090311	1
Klenk	Chicory root	6221N130201	1
Klenk	Chicory root	A130304	1
Klenk	Chicory root	6221A130304	1
Kräuter Schulte	China Pai Mu Tan	52783	1
Fagron	Chlorhexidine dihydrochloride	14A09B03	1
Fagron	Chlorhexidine dihydrochloride	14A09-B03-293425	1
Euro OTC	Cholecalciferol dry concentrate	1012025-01	1
Euro OTC	Cholecalciferol dry concentrate	1602019-02	5
Euro OTC	Cholecalciferol dry concentrate	1608002-01	15
Euro OTC	Cholecalciferol dry concentrate	1508032-01	2
Euro OTC	Cholecalciferol dry concentrate	1701053-01	11
Euro OTC	Cholecalciferol dry concentrate	150803201	1
Euro OTC	Cholecalciferol dry concentrate	1707027-01	17

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Euro OTC	Cholecalciferol dry concentrate	1801038-01	4
Euro OTC	Cholecalciferol dry concentrate	1802014-01	17
Euro OTC	Cholecalciferol dry concentrate	170153-01	5
Euro OTC	Cholecalciferol dry concentrate	1806003-01	28
Euro OTC	Cholecalciferol dry concentrate	2001007-01	1
Euro OTC	Cholecalciferol dry concentrate	1502021-01	1
Euro OTC	Cholecalciferol dry concentrate	1901050-01	4
Euro OTC	Cholecalciferol dry concentrate	1906009-01	8
Euro OTC	Cholecalciferol dry concentrate	1906009-02	5
Euro OTC	Cholecalciferol dry concentrate	1210051-01	1
Euro OTC	Cholecalciferol dry concentrate	1602019-01	2
Euro OTC	Cholecalciferol dry concentrate	L1403012-01	1
Euro OTC	Cholecalciferol dry concentrate	1806003-02	1
Euro OTC	Chromium yeast 0.2%	L1311026-01	1
Fagron	Cinchocaine hydrochloride	12F25-N10	1
Phönix	Cinchocaine hydrochloride	13E13-N07	1
Caelo	Cinchona bark, cut	10381906	1
Caelo	Cinchona bark, cut	15301904	2
Caelo	Cinchona bark, cut	14009305	1
Klenk	Cinchona bark, cut	601B130415	1
Klenk	Cinchona bark, cut	601B130415	1
Akazie	Cinnamon	20.09.2015	1
Akazien-Apo	Cinnamon	Test	1
Caelo	Cinnamon	11357909	1
Caelo	Cinnamon	11357912	2
Caelo	Cinnamon	12309902	3
Caelo	Cinnamon	12309908	1
Caelo	Cinnamon	25111307	1
Caelo	Cinnamon	12309909	1
Caelo	Cinnamon	13304401	2
Caelo	Cinnamon	13304415	1
Caelo	Cinnamon	13304402	2
Caelo	Cinnamon	13304409	1
Caelo	Cinnamon	13304407	1
Caelo	Cinnamon	15151905	1
Caelo	Cinnamon	16061702	1
Fargon / Gehe	Cinnamon	15104201	1
Caelo	Cinnamon	15151902	1
Caelo	Cinnamon	16245105	1
Klenk	Cinnamon	610A101018	1
Klenk	Cinnamon	610A130927	1
siehe Protokoll	Cinnamon	sieheProtokoll	1
Caelo	Cinnamon rods (Ceylonese Ci…	12148904	1
Klenk	Cinnamon rods (Ceylonese Ci…	A101018	1
Klenk	Cinnamon rods (Ceylonese Ci…	B121016	1
Klenk	Cinnamon rods (Ceylonese Ci…	610A101018	1
Phönix	Cinnamon rods (Ceylonese Ci…	610A130927	1
Sanacorp	Cinnamon rods (Ceylonese Ci…	13231601	1
Fagron	Cinnarizine	13H01-N07	4
Fagron	Cinnarizine	14D09-B01-292883	1
Fagron	Cinnarizine	14D09-B01	3
Fagron	Cinnarizine	8D11-N04	1
Fagron	Cinnarizine	13I26-N22	1
Fagron	Cinnarizine	13I26-N22	1
Fagron	Clobetasol-17-propionate 1:…	12A03-N03	1
Fagron	Clobetasol-17-propionate 1:…	11k04-n17	1
Fagron	Clobetasol-17-propionate 1:…	12|19-N01	1
Fagron	Clobetasol-17-propionate 1:…	12l19-N01	1
Fagron	Clobetasol-17-propionate 1:…	12I19-N01	2
Fagron	Clobetasol-17-propionate 1:…	12K08-N02	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Clobetasol-17-propionate 1:...	13W16-N01	1
Fagron	Clobetasol-17-propionate 1:...	12L19-N06	1
Fagron	Clobetasol-17-propionate 1:...	12/19-No1	1
Fagron	Clobetasol-17-propionate 1:...	12/19-N01003637	1
Caelo	Clove	5398872	1
Caelo	Clove	12095802	1
Caelo	Clove	11233305	1
Caelo	Clove	12095807	5
Caelo	Clove	12095806	2
Caelo	Clove	12266505	1
Caelo	Clove	13371309	1
Caelo	Clove	16207802	1
Caelo	Clove	14057602	1
Klenk	Clove	1260A110608	5
Klenk	Clove	1260A100617	2
Klenk	Clove	1260A101223	1
Klenk	Clove	A120328	1
Klenk	Clove	1260A120328	6
Klenk	Clove	1260A130903	3
Klenk	Clove	1260A150304	2
Caelo	Clove, powdered (spice)	14180001	1
Caelo	Clove, powdered (spice)	12355303	1
	Cocaine hydrochloride	21004044019	1
Caelo	Cocaine hydrochloride	12329103	1
Caelo	Cocaine hydrochloride	13259306	1
Caelo	Cocaine hydrochloride	14069209	1
Caelo	Cocaine hydrochloride	17003902	4
Caelo	Cocaine hydrochloride	18J01-B07-353630	2
Caelo	Cocaine hydrochloride	18266109	3
Caelo	Cocaine hydrochloride	18256109	1
Caelo	Cocaine hydrochloride	19073003	1
Caelo	Cocaine hydrochloride	20003901001	2
Caelo	Cocaine hydrochloride	21004044004	1
Caelo	Cocaine hydrochloride	17003909	1
Caelo	Cocaine hydrochloride	13112102	1
Caesar & Loretz GmbH	Cocaine hydrochloride	182661001	1
Caesar & Loretz GmbH	Cocaine hydrochloride	21004044009	1
Caesar & Loretz Gm...	Cocaine hydrochloride	18266104	4
Caesar & Loretz Gm...	Cocaine hydrochloride	182661	1
Fagron	Cocaine hydrochloride	12G23-N13	1
Fagron	Cocaine hydrochloride	13G03-N08	2
Fagron	Cocaine hydrochloride	14H27-B03	1
Fagron	Cocaine hydrochloride	15E12-B03	1
Fagron	Cocaine hydrochloride	16B11-B05-323385	1
Fagron	Cocaine hydrochloride	17E17-B07-335110	1
Fagron	Cocaine hydrochloride	15-00638	1
Fagron	Cocaine hydrochloride	17K28-B05-343075	1
Fagron	Cocaine hydrochloride	21K30-F04	1
Fagron	Cocaine hydrochloride	18J01-B07-353629	1
Gatt-Koller	Cocaine hydrochloride	20172282	1
Macfarlan Smith/Noweda	Cocaine hydrochloride	15224802	2
Caelo	Cocaine hydrochloride	16051402	1
Synopharm	Cocaine hydrochloride	16B11-B05	1
Caelo	Cocoa bark, cut	19011303	1
Caelo	Cocoa bark, cut	12126901	1
Caelo	Cocoa bark, cut	12126907	1
Caelo	Cocoa bark, cut	12126910	1
Caelo	Cocoa bark, cut	12126905	2
Caelo	Cocoa bark, cut	1216907	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caeleo/ Kehr	Codeine phosphate hemihydrate	181879001	2
Caelo	Codeine phosphate hemihydrate	15350703	2
Caelo	Codeine phosphate hemihydrate	17160503	3
Caelo	Codeine phosphate hemihydrate	18187903	5
Caelo	Codeine phosphate hemihydrate	18187960	2
Caelo	Codeine phosphate hemihydrate	181817907	1
Caelo	Codeine phosphate hemihydrate	16169805	3
Caelo	Codeine phosphate hemihydrate	14275910	1
Caelo	Codeine phosphate hemihydrate	18187907	1
Caelo	Codeine phosphate hemihydrate	15219805	2
Caelo	Codeine phosphate hemihydrate	16349708	2
Caelo	Codeine phosphate hemihydrate	18187908	1
Caelo	Codeine phosphate hemihydrate	1427910	1
Caelo	Codeine phosphate hemihydrate	20003804005	1
Caelo	Codeine phosphate hemihydrate	13I27-N06	1
Caelo	Codeine phosphate hemihydrate	16349704	2
Caelo	Codeine phosphate hemihydrate	16349707	1
Caelo	Codeine phosphate hemihydrate	17L22-B03-343752	2
Caelo	Codeine phosphate hemihydrate	20003804007	1
Caesar & Loretz GmbH	Codeine phosphate hemihydrate	18187906	5
Caesar & Loretz GmbH	Codeine phosphate hemihydrate	18187902	4
Caesar & Loretz GmbH	Codeine phosphate hemihydrate	18187901	1
Euro OTC	Codeine phosphate hemihydrate	CP04236	1
Euro/ Sanacorp	Codeine phosphate hemihydrate	15F09-B02-315564	2
Fagron	Codeine phosphate hemihydrate	11/19-N10	1
Fagron	Codeine phosphate hemihydrate	12C05-N01	1
Fagron	Codeine phosphate hemihydrate	13E21-N04	1
Fagron	Codeine phosphate hemihydrate	13C11-N10	1
Fagron	Codeine phosphate hemihydrate	1615I-01279	1
Fagron	Codeine phosphate hemihydrate	13/27-N06	2
Fagron	Codeine phosphate hemihydrate	15B17-B99-304623	2
Fagron	Codeine phosphate hemihydrate	15F09-B02-310520	2
Fagron	Codeine phosphate hemihydrate	21D30-F01-380923	1
Fagron	Codeine phosphate hemihydrate	B01-3612302	2
Fagron	Codeine phosphate hemihydrate	15F09-B02	1
Fagron	Codeine phosphate hemihydrate	15F09-B02-314033	1
Fagron	Codeine phosphate hemihydrate	16E17-B05-324109	4
Fagron	Codeine phosphate hemihydrate	18D03-B01	1
Fagron	Codeine phosphate hemihydrate	5040218D	3
Fagron	Codeine phosphate hemihydrate	21D30-F01	1
Fagron	Codeine phosphate hemihydrate	F04-3825805	1
Fagron	Codeine phosphate hemihydrate	913I-01279	1
Gehe	Codeine phosphate hemihydrate	15350710	3
Merck	Codeine phosphate hemihydrate	120765	1
Caelo	Codeine phosphate hemihydrate	16349706	2
Caelo	Codeine phosphate hemihydrate	130715	1
Th. Geyer	Codeine phosphate hemihydrate	67038	1
Th. Geyer	Codeine phosphate hemihydrate	70533	22
Th. Geyer	Codeine phosphate hemihydrate	67054	31
Fagron	Colophony	15186807	8
Bombastus	Coltsfoot leaf	277848	2
Bombastus	Coltsfoot leaf	269501	3
Bombastus	Coltsfoot leaf	272019	1
Bombastus	Coltsfoot leaf	276303	5
Bombastus	Coltsfoot leaf	285263	3
Bombastus	Coltsfoot leaf	265856	1
Bombastus	Coltsfoot leaf	274289	5
Bombastus	Coltsfoot leaf	275489	3
Bombastus	Coltsfoot leaf	281100	4
Bombastus	Coltsfoot leaf	277131	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Coltsfoot leaf	232339	1
Bombastus	Coltsfoot leaf	278758	7
Caelo	Coltsfoot leaf	23041302	1
Caelo	Coltsfoot leaf	Int.Ch:Now16081	1
Gehe	Coltsfoot leaf	2021B121204	9
Klenk	Coltsfoot leaf	8061207	1
Klenk	Coltsfoot leaf	11101202	1
Klenk	Coltsfoot leaf	2021B120124	4
Klenk	Coltsfoot leaf	2021B120601	5
Klenk	Coltsfoot leaf	5011301	1
Klenk	Coltsfoot leaf	20021301	1
Klenk	Coltsfoot leaf	KS100061	1
Klenk	Coltsfoot leaf	2021B130319	4
Klenk	Coltsfoot leaf	B120124	1
Klenk	Coltsfoot leaf	26091301	1
Klenk	Coltsfoot leaf	14111302	1
Klenk	Coltsfoot leaf	5122013a	1
Klenk	Coltsfoot leaf	23121302	1
Klenk	Coltsfoot leaf	B130227	1
Klenk	Coltsfoot leaf	2021C140730	1
Klenk	Coltsfoot leaf	2021B150407	1
Klenk	Coltsfoot leaf	2020B120124	1
Klenk	Coltsfoot leaf	2021B130227	12
Klenk	Coltsfoot leaf	2021B111005	1
Klenk	Coltsfoot leaf	2021B140131	1
Klenk	Coltsfoot leaf	2021b121204	1
Klenk	Coltsfoot leaf	2021C130326	8
Noweda	Coltsfoot leaf	2021B111111	3
Phönix	Coltsfoot leaf	278296	4
Klenk	Coltsfoot leaf	2021B121203	5
Bombastus	Comfrey herb, cut	281531	1
Klenk	Comfrey herb, cut	4561B100518	2
Caelo	Comfrey root	2711Q-02135	1
Caelo	Comfrey root	116053	1
Hof-Apotheke,St.Afra	Comfrey root	125041	1
Klenk	Comfrey root	6241B120531	3
Klenk	Comfrey root	6241B120807	4
Klenk	Comfrey root	6241B100715	1
Klenk	Comfrey root	6241B130619	8
Klenk	Comfrey root	B130619	1
Klenk	Comfrey root	6241B130724	7
Klenk	Comfrey root	6241B131009	1
Klenk	Comfrey root	6241B121214	2
Klenk	Comfrey root	6244B130624	1
Klenk	Comfrey root	6241B06110202	1
Klenk	Comfrey root	6241B130312	3
Klenk	Comfrey root	6241b130619	1
Klenk	Comfrey root	6241b130724	1
Klenk	Comfrey root	6241b120807	1
Caelo	Common broom herb, cut	11132209	1
Caelo	Common broom herb, cut	4412Q-01680	1
Caelo	Common broom herb, cut	12358802	1
Caelo	Common broom herb, cut	12358804	3
Caelo	Common broom herb, cut	12358805	1
Caelo	Common broom herb, cut	13241601	1
Galke	Common broom herb, cut	12358803	4
Phönix	Common broom herb, cut	12358801	2
AHD	Common wormwood herb	521603580	1
AHD	Common wormwood herb	16310701	1
Caelo	Common wormwood herb	12016708	5

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Aurica	Common wormwood herb	521305386	1
Caelo	Common wormwood herb	12016702	1
Caelo	Common wormwood herb	3591A110119	4
Caelo	Common wormwood herb	12016705	5
Caelo	Common wormwood herb	12016707	3
Caelo	Common wormwood herb	18031302	1
Caelo	Common wormwood herb	1081301	1
Caelo	Common wormwood herb	12382702	12
Caelo	Common wormwood herb	12382705	2
Caelo	Common wormwood herb	12382706	1
Caelo	Common wormwood herb	14360605	1
Caelo	Common wormwood herb	12016709	2
Caelo	Common wormwood herb	12016711	3
Caelo	Common wormwood herb	12382701	7
Caelo	Common wormwood herb	9355403	1
Galke	Common wormwood herb	21637	1
Caelo	Common wormwood herb	10355329	1
Caelo	Common wormwood herb	1238701	1
Klenk	Common wormwood herb	3591A120123	8
Klenk	Common wormwood herb	A120123	2
Klenk	Common wormwood herb	3591A130218	10
Klenk	Common wormwood herb	3591a130218	2
Klenk	Common wormwood herb	3591a120123	1
Klenk	Common wormwood herb	2591A130218	1
Klenk	Common wormwood herb	3591A11119	1
Richter	Common wormwood herb	b200112	1
Caelo	Copper(II) sulfate pentahydrate	3411M-01317	1
Caelo	Copper(II) sulfate pentahydrate	12157107	1
Caelo	Copper(II) sulfate pentahydrate	10L15-N06	1
Caelo	Copper(II) sulfate pentahydrate	3211M-01317	1
Caelo	Copper(II) sulfate pentahydrate	2913U-01317	1
Fagron	Copper(II) sulfate pentahydrate	13A25-N06	1
Bombastus	Coriander	263733	1
Bombastus	Coriander	306310	1
Caelo	Coriander	13010304	1
Caelo	Coriander	12080901	2
Caelo	Coriander	14031316	1
Caelo	Coriander	13010302	2
Caelo	Coriander	27061305	1
Caelo	Coriander	4091305	1
Caelo	Coriander	13010306	2
Caelo	Coriander	16010209	1
Caelo	Coriander	12080906	1
Caelo	Coriander	9285707	1
Caelo	Coriander	16010201	1
Caesar/Noweda	Coriander	2010M-01539	1
Klenk	Coriander	2790A161111	5
Caelo	Coriander	12080905	1
Klenk	Coriander	2790A121023	7
Klenk	Coriander	A121023	3
Klenk	Coriander	2790A130129	2
Klenk	Coriander	2709A130129	1
Klenk	Coriander	2790A151117	1
Klenk	Coriander	2790a121023	1
Caelo	Coriander	18010209	1
sanacorp;3,32;18.06.15	Coriander	13299495	1
Caelo	Cottonwood bud	12027506	1
Caelo	Cottonwood bud	70864257	1
Klenk	Cottonwood bud	3260A120828	1
Caelo	Cottonwood bud	12027504	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Couch grass rhizome, cut	276777	3
Bombastus	Couch grass rhizome, cut	273387	3
Bombastus	Couch grass rhizome, cut	270500	2
Bombastus	Couch grass rhizome, cut	278926	1
Bombastus	Couch grass rhizome, cut	262175	1
Caelo	Couch grass rhizome, cut	10049614	1
Caelo	Couch grass rhizome, cut	10049618	2
Caelo	Couch grass rhizome, cut	10349705	1
Caelo	Couch grass rhizome, cut	10349704	1
Caelo	Couch grass rhizome, cut	3712I-02180	1
Caelo	Couch grass rhizome, cut	12186817	3
Caelo	Couch grass rhizome, cut	12186705	1
Caesar/Noweda	Couch grass rhizome, cut	12186813	4
Galke	Couch grass rhizome, cut	18781	1
Gehe	Couch grass rhizome, cut	12186704	1
Gehe	Couch grass rhizome, cut	283061	1
Kräuter Schulte	Couch grass rhizome, cut	53016	2
Caelo	Cowberry leaf, cut	12105201	1
Caelo	Cowberry leaf, cut	12105203	1
Caelo	Cowberry leaf, cut	12150205	1
Caelo	Cowberry leaf, cut	11334302	1
Klenk	Cowberry leaf, cut	2431B101006	2
Creapure	Creatine	515941	1
Degussa / falcento	Creatine	422031	1
Phönix	Creatine	mysjhskeu	1

D

Supplier	Substance	Batch	Spectra
Falcento	D-(+)-mannose	R-4638	1
Falcento	D-(+)-mannose	R-4639	1
Falcento	D-(+)-mannose	R4640	1
Falcento	D-(+)-mannose	R-4641	1
Giusto Faravelli	D-(+)-mannose	161004/1710215001	1
Caelo	Daisy flower	11103201	2
Caelo	Daisy flower	11068308	1
Caelo	Daisy flower	1210a120215	2
Caelo	Daisy flower	12133703	1
Caelo	Daisy flower	12133704	1
Caelo	Daisy flower	12133705	1
Caelo	Daisy flower	11103203	2
Hepart AG	Daisy flower	A130307	1
Kenk / Phoenix	Daisy flower	1210A130307	4
Klenk	Daisy flower	A130705	1
Klenk	Daisy flower	1210A110223	1
Klenk	Daisy flower	1210A120215	4
Klenk	Daisy flower	1210a071301	1
Klenk	Damiana leaf, cut	12064101	1
Caelo	Damiana leaf, cut	12330402	7
Caelo	Damiana leaf, cut	12330403	2
Caelo	Damiana leaf, cut	12330401	5
Caelo	Damiana leaf, cut	12064103	3
Caelo	Damiana leaf, cut	11026607	2
Caelo	Damiana leaf, cut	12330407	2
Klenk	Damiana leaf, cut	A130206	2
Klenk	Damiana leaf, cut	1990A130206	1
Noweda	Damiana leaf, cut	200151	1
Redwood	Damiana leaf, cut	216451	1
Anzag	Dandelion herb with root	274030	1
Anzag 10.05.13 ek:3,16EUR	Dandelion herb with root	6611B130321	1

continued on the next page

continued from previous page

Supplier		Substance	Batch	Spectra
Anzag ek:3.16EUR	25.10.12	Dandelion herb with root	6611B110131	1
Aurica		Dandelion herb with root	521200197	1
Bombastus		Dandelion herb with root	258809	1
Bombastus		Dandelion herb with root	271272	5
Bombastus		Dandelion herb with root	274030	5
Bombastus		Dandelion herb with root	280363	5
Bombastus		Dandelion herb with root	285264	1
Bombastus		Dandelion herb with root	290125	1
Bombastus		Dandelion herb with root	275126	1
Bombastus		Dandelion herb with root	280363-3385310110	1
Bombastus		Dandelion herb with root	282916	7
Caelo		Dandelion herb with root	20111202	1
Caelo		Dandelion herb with root	13108801	4
Caelo		Dandelion herb with root	11030309	2
Caelo		Dandelion herb with root	806212165	1
Caelo		Dandelion herb with root	8111205	1
Caelo		Dandelion herb with root	12236003	3
Caelo		Dandelion herb with root	12236002	8
Caelo		Dandelion herb with root	2112122165	1
Caelo		Dandelion herb with root	11371903	1
Caelo		Dandelion herb with root	11030305	1
Caelo		Dandelion herb with root	13019802	19
Caelo		Dandelion herb with root	13018902	1
Caelo		Dandelion herb with root	Int.Ch:318090	1
Caelo		Dandelion herb with root	13199202	2
Caelo		Dandelion herb with root	17121305	1
Caelo		Dandelion herb with root	13317903	1
Caelo		Dandelion herb with root	Ch.-B.:13019802	1
Caelo		Dandelion herb with root	11030313	2
Caelo		Dandelion herb with root	12236001	3
Caelo		Dandelion herb with root	6611B100902	1
Caelo		Dandelion herb with root	18035117	1
Caelo		Dandelion herb with root	19114404	1
Caelo		Dandelion herb with root	19114406	1
Caelo		Dandelion herb with root	13019805	1
Caelo		Dandelion herb with root	13019802-3395310101	1
Caelo		Dandelion herb with root	12236005	5
Caelo		Dandelion herb with root	1103011	1
Caelo		Dandelion herb with root	13019801	5
Caelo		Dandelion herb with root	11030311	2
Caelo		Dandelion herb with root	11030314	4
Caelo		Dandelion herb with root	13108802	11
Caelo		Dandelion herb with root	18046901	1
Caelo		Dandelion herb with root	7341703	1
Caelo		Dandelion herb with root	18035103	1
Caelo		Dandelion herb with root	18035108	3
Caelo		Dandelion herb with root	18035113	1
Euro OTC		Dandelion herb with root	11030312	4
Galke		Dandelion herb with root	20531	6
Galke		Dandelion herb with root	22093	2
Gehe		Dandelion herb with root	6611B110104	1
Gehe		Dandelion herb with root	13019803	1
Hedinger		Dandelion herb with root	10121614	1
Klenk		Dandelion herb with root	6611B110131	1
Klenk		Dandelion herb with root	6611B160613	1
Klenk		Dandelion herb with root	6611B120620	19
Klenk		Dandelion herb with root	6611A110104	1
Klenk		Dandelion herb with root	6611B130314	3
Klenk		Dandelion herb with root	5122013b	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Dandelion herb with root	6611B1104104	1
Klenk	Dandelion herb with root	6611B090306	1
Klenk	Dandelion herb with root	6611B-120620	1
Klenk	Dandelion herb with root	6611B-131206	1
Klenk	Dandelion herb with root	6611B110104	5
Klenk	Dandelion herb with root	6611B110929	2
Bombastus	Dandelion herb with root	277597	6
Phönix	Dandelion herb with root	6611B130321	29
Sanacorp	Dandelion herb with root	13108803	2
Caelo	Dandelion herb with root	10121602	1
Caelo	Dandelion herb without root	11217107	1
Caelo	Dandelion herb without root	11030311	1
Caelo	Dandelion herb without root	11217109	2
Caelo	Dandelion herb without root	7031305	1
Caelo	Dandelion herb without root	11371904	2
Caelo	Dandelion herb without root	1127102	1
Caelo	Dandelion herb without root	13091305	1
Caelo	Dandelion herb without root	11371907	1
Caelo	Dandelion herb without root	11371902	1
Caelo	Dandelion herb without root	1137907	1
Caelo	Dandelion herb without root	9011403	1
Caelo	Dandelion herb without root	107063	1
Caelo	Dandelion root	12363104	3
Caelo	Dandelion root	10024710	1
Caelo	Dandelion root	11003307	1
Caelo	Dandelion root	11003311	2
Caelo	Dandelion root	12363102	2
Caelo	Dandelion root	12363103	1
Caelo	Dandelion root	12363107	1
Caelo	Dandelion root	12367916	1
Caelo	Dandelion root	12363109	2
Caelo	Dandelion root	12363108	2
Caelo	Dandelion root	12363110	1
Caelo	Dandelion root	13329705	1
Caelo	Dandelion root	13329708	1
Caelo	Dandelion root	14166502	1
Caelo	Dandelion root	15096601	1
Caelo	Dandelion root	15407703	1
Caelo	Dandelion root	16161308	1
Caelo	Dandelion root	15407703	1
Caelo	Dandelion root	13329702	10
Caelo	Dandelion root	16161303	1
Caelo	Dandelion root	14166504	1
Caelo	Dandelion root	14376602	1
Caelo	Dandelion root	12363106	1
Caelo	Dandelion root	11003313	1
Caelo	Dandelion root	14166501	1
Caelo	Dandelion root	14376603	1
Galke	Dandelion root	126302	1
Galke	Dandelion root	20658	1
Caelo	Dandelion root	1140317	1
Klenk	Dandelion root	6621A120208	6
Klenk	Dandelion root	6621A110420	1
Klenk	Dandelion root	6101202	1
Klenk	Dandelion root	A120606	1
Klenk	Dandelion root	N130813	1
Klenk	Dandelion root	6621A160111	2
Klenk	Dandelion root	6621B170112	1
Klenk	Dandelion root	6621N130813	6
Klenk	Dandelion root	6621A140114	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Dandelion root	6621A140114	3
Klenk	Dandelion root	6621A120606	15
Klenk	Dandelion root	6621A141027	5
noweda	Dandelion root		1
Caelo	Dapsone	18279201	4
Caelo	Dapsone	17031101	2
Caelo	Dapsone	19113501	3
Caesar & Loretz GmbH	Dapsone	191135001	1
Euro OTC	Deoxycholic acid	1305051-01	1
Fagron	Deoxycholic acid	13J21-N14	1
Gehe	Deoxycholic acid	2012060253	1
GEHE 21.10.2014	Deoxycholic acid	13F13-N06	1
Caelo	Devil's claw root	12031806	1
Caelo	Devil's claw root	12031810	1
Caelo	Devil's claw root	12031809	1
Caelo	Devil's claw root	12031811	1
Caelo	Devil's claw root	6331B110426	2
Caelo	Devil's claw root	12031803	1
Galke	Devil's claw root	20282	2
Galke	Devil's claw root	21018	2
Gehe	Devil's claw root	1114005	1
Klenk	Devil's claw root	10111204	1
Klenk	Devil's claw root	6331B130129	5
Klenk	Devil's claw root	6331B120508	3
Caelo	Dexamphetamine sulfate	C9H13N14	1
Fagron	Dexamphetamine sulfate	11F29-N01	1
Fagron	Dexamphetamine sulfate	17B09-B02-339690	1
Fagron	Dexamphetamine sulfate	20D10-F02-370502	1
Fagron	Dexamphetamine sulfate	22A18-F01-383285	1
Fagron	Dexamphetamine sulfate	17B09-B02-339689	4
Fagron	Dexamphetamine sulfate	B50-3632406	2
Fagron	Dexamphetamine sulfate	F02-3705003	2
Fagron	Dexamphetamine sulfate	F01-3764108	1
Fagron	Dexamphetamine sulfate	22A18-F01-383287	2
Fagron	Dexamphetamine sulfate	15H06-B04-313861	1
Fagron	Dexamphetamine sulfate	19D12-B50-363247	6
Fagron	Dexamphetamine sulfate	20D10-F02-370503	1
Fagron	Dexamphetamine sulfate	20D10-F02_370503	1
Fagron	Dexamphetamine sulfate	20D10-F02	3
Fagron	Dexamphetamine sulfate	16F09-B02-328352	1
Fagron	Dexamphetamine sulfate	17B019-B02-339689	1
Fagron	Dexamphetamine sulfate	17B09-B02	2
Fagron	Dexamphetamine sulfate	19D12-B50	2
Fagron	Dexamphetamine sulfate	19D12-B50-363246	3
Fargon/ Phönix	Dexamphetamine sulfate	F000876	1
Fargon/Gehe	Dexamphetamine sulfate	15H06-B04	1
	Dihydrocodeine hydrogen tartrate	21F03-F02-379260	3
	Dihydrocodeine hydrogen tartrate	3020321	2
Caelo	Dihydrocodeine hydrogen tartrate	12142503	2
Caelo	Dihydrocodeine hydrogen tartrate	12142508	2
Caelo	Dihydrocodeine hydrogen tartrate	13267603	1
Caelo	Dihydrocodeine hydrogen tartrate	13267604	2
Caelo	Dihydrocodeine hydrogen tartrate	13267608	1
Caelo	Dihydrocodeine hydrogen tartrate	15295903	2
Caelo	Dihydrocodeine hydrogen tartrate	16106202	5
Caelo	Dihydrocodeine hydrogen tartrate	15F18-B07-322054	1
Caelo	Dihydrocodeine hydrogen tartrate	18115205	2
Caelo	Dihydrocodeine hydrogen tartrate	15295905	4
Caelo	Dihydrocodeine hydrogen tartrate	15295907	1
Caelo	Dihydrocodeine hydrogen tartrate	16106203	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dihydrocodeine hydrogen tartrate	17097508	2
Caelo	Dihydrocodeine hydrogen tartrate	18115202	3
Caelo	Dihydrocodeine hydrogen tartrate	19D15-B02-363307	1
Caesar & Loretz GmbH	Dihydrocodeine hydrogen tartrate	192004005	1
Caesar & Loretz GmbH	Dihydrocodeine hydrogen tartrate	20003430003	1
Caesar & Loretz GmbH	Dihydrocodeine hydrogen tartrate	20003430006	1
Fagron	Dihydrocodeine hydrogen tartrate	12G05-N01	1
Fagron	Dihydrocodeine hydrogen tartrate	13H19-N08	3
Fagron	Dihydrocodeine hydrogen tartrate	14D08-B06	1
Fagron	Dihydrocodeine hydrogen tartrate	14K26-B04	1
Fagron	Dihydrocodeine hydrogen tartrate	14K26-B04-317257	1
Fagron	Dihydrocodeine hydrogen tartrate	15F18-B07	1
Fagron	Dihydrocodeine hydrogen tartrate	15F18-B07-323388	1
Fagron	Dihydrocodeine hydrogen tartrate	15F18B07	2
Fagron	Dihydrocodeine hydrogen tartrate	16I27-B03-332122	1
Fagron	Dihydrocodeine hydrogen tartrate	16-00326	1
Fagron	Dihydrocodeine hydrogen tartrate	16I27-B03	1
Fagron	Dihydrocodeine hydrogen tartrate	17G04-B02-342861	1
Fagron	Dihydrocodeine hydrogen tartrate	17G04-B02	1
Fagron	Dihydrocodeine hydrogen tartrate	3080620	1
Fagron	Dihydrocodeine hydrogen tartrate	21f03-f02-379260	1
Fagron	Dihydrocodeine hydrogen tartrate	14K26-B04-310974	1
Fagron	Dihydrocodeine hydrogen tartrate	B02-3683109	1
Fagron	Dihydrocodeine hydrogen tartrate	F02-3756503	4
Caelo	Dihydrocodeine hydrogen tartrate	17097502	2
Th. Geyer	Dihydrocodeine hydrogen tartrate	70729	6
Hedinger	Dihydrocodeine hydrogen tartrate	70162	4
Th. Geyer	Dihydrocodeine hydrogen tartrate	59819	1
Th. Geyer	Dihydrocodeine hydrogen tartrate	67052	10
Th. Geyer	Dihydrocodeine hydrogen tartrate	20170808-03065	1
Th. Geyer	Dihydrocodeine hydrogen tartrate	67035	2
Akazie	Dill fruit	20.09.2015	1
Caelo	Dill fruit	12289901	1
Caelo	Dill fruit	12038302	2
Caelo	Dill fruit	12342901	2
Caelo	Dill fruit	12342904	7
Caelo	Dill fruit	12342903	1
Caelo	Dill fruit	12342908	2
Caelo	Dill fruit	12038304	4
Caelo	Dill fruit	9189003	1
Caelo	Dill fruit	16040406	1
Caelo	Dill fruit	12342906	2
Galke	Dill fruit	22422	4
Hepart AG	Dill fruit	L30057kbA	1
Klenk	Dill fruit	2680A-120312	1
Klenk	Dill fruit	2680A120312	8
Klenk	Dill fruit	A120312	1
Klenk	Dill fruit	2680A121211	3
Klenk	Dill fruit	2680a120312	1
Kräuter Schulte	Dill fruit	6363	1
Caelo	Dill fruit	16348702	2
Caelo	Dill fruit	16348707	1
Caelo	Dill fruit	12342909	5
Wolf	Dill fruit	E-501	1
Wolf	Dill fruit	L30057	5
Wolf	Dill fruit	23622	6
Bombastus	Dill herb, cut	50836505	1
Caelo	Dill herb, cut	11295109	1
Caelo	Dill herb, cut	13007601	1
Caelo	Dill herb, cut	13007605	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Dill herb, cut	15178603	1
Caelo	Dill herb, cut	13007602	1
Caelo	Dill herb, cut	13007608	1
Klenk	Dill herb, cut	3531B110726	1
Dr. Behr	Dimercaptosuccinic acid	WE14020002	1
Lab.Offichem	Dimethyl fumarate	1605052.0393	1
Lab.Offichem	Dimethyl fumarate	1805043.0393	1
Lab.Offichem	Dimethyl fumarate	1808016.0393	1
Lab.Offichem	Dimethyl fumarate	1809012.0393	1
Lab.Offichem	Dimethyl fumarate	1910037.1814	1
Falcento	D-Ribose	201206712	2
Falcento	D-Ribose	201209702	1
Falcento	D-Ribose	JXCZSJ14-D-010	1
Unisan	D-Ribose	JXCZSJ13D-013	2
Fagron	Drofenine hydrochloride	12D04-N03	1
Fagron	Drofenine hydrochloride	11J24-N01	1
Caelo	Dry beads Caelo orange	11005811	1
Kräuter Schulte	Dryas octopetala herb, cut	38970	1

E

Supplier	Substance	Batch	Spectra
Caelo	Econazole nitrate	ECN140301	1
Fagron	Econazole nitrate	11K07-N03	1
Fagron	Econazole nitrate	13D22-N06	1
Fagron	Econazole nitrate	11F09-N16	1
Fagron	Econazole nitrate	12F18-N05	1
Fagron	Econazole nitrate	14G22-B07-306926	1
Caelo	Elder berries	12267801	1
Gehe	Elder berries	12267807	1
Klenk	Elder berries	3010N120921	3
Bombastus	Elder flower	275393	4
Bahnhof-Apotheke	Elder flower	17-121112	1
Bombastus	Elder flower	265631	1
Bombastus	Elder flower	289348	1
Bombastus	Elder flower	279216	3
Caelo	Elder flower	12221902	11
Caelo	Elder flower	10291308	2
Caelo	Elder flower	10291312	2
Caelo	Elder flower	12221904	10
Caelo	Elder flower	1571a121022	1
Caelo	Elder flower	31051301	1
Caelo	Elder flower	12221905	7
Caelo	Elder flower	12221906	1
Caelo	Elder flower	12221907	4
Caelo	Elder flower	14111317	1
Caelo	Elder flower	5122013d	1
Caelo	Elder flower	12221909	1
Caelo	Elder flower	13244601	4
Caelo	Elder flower	13244602	2
Caelo	Elder flower	12221910	2
Caelo	Elder flower	1571A121022	14
Caelo	Elder flower	10291309	3
Caelo	Elder flower	12221904-3360319071	1
Caesar/Noweda	Elder flower	4910A-01471	1
Finze	Elder flower	9297415	1
Galke	Elder flower	21934	1
Gehe	Elder flower	1250213	1
Gehe	Elder flower	1090413	1
Klenk	Elder flower	1571A141126	1
Klenk	Elder flower	1571A110223	16

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Elder flower	16061201	1
Klenk	Elder flower	26061201	1
Klenk	Elder flower	21091201	1
Klenk	Elder flower	1571A110125	2
Klenk	Elder flower	13021301	1
Klenk	Elder flower	1571A121121	20
Klenk	Elder flower	1571A1202015	1
Klenk	Elder flower	A121121	1
Klenk	Elder flower	A120215	1
Klenk	Elder flower	1571A130627	2
Klenk	Elder flower	1571A-110223	1
Klenk	Elder flower	1571a120215	1
Klenk	Elder flower	1571A130930	3
Klenk	Elder flower	1571a1211	1
Klenk	Elder flower	1571A120215	4
Caelo	Elder flower	1029310	1
Bombastus	Elder flower	269873	2
Caelo	Elder flower	10291310	5
Wolf	Elder flower	E-738	1
Wolf	Elder flower	22749	1
Wolf	Elder flower	22765	1
Wolf	Elder flower	B-810	1
Klenk	Elder root, cut	6281B110427	4
Probe	Elder root, cut	12345	1
-	Elecampane rhizome, cut	712M-02181	1
Caelo	Elecampane rhizome, cut	12113304	3
Caelo	Elecampane rhizome, cut	1211334	1
Caelo	Elecampane rhizome, cut	6341B	1
Caelo	Elecampane rhizome, cut	11374702	1
Caelo	Elecampane rhizome, cut	13152402	1
Caelo	Elecampane rhizome, cut	13152401	1
Caelo	Elecampane rhizome, cut	12113303	1
Galke	Elecampane rhizome, cut	21569	2
Gehe	Elecampane rhizome, cut	11196906	1
Gehe	Elecampane rhizome, cut	12113302	2
Caelo	Elecampane rhizome, cut	11374703	1
Klenk	Elecampane rhizome, cut	6341B100426	2
Klenk	Elecampane rhizome, cut	6341B120611	2
Klenk	Elecampane rhizome, cut	B130423	3
Klenk	Elecampane rhizome, cut	6341B130423	3
Klenk	Elecampane rhizome, cut	6311141B130423	1
Noweda	Elecampane rhizome, cut	6341B111118	3
Caelo	Elecampane rhizome, cut	13152403	2
Richter	Elecampane rhizome, cut	P158683	1
Caelo	Eleutherococcus, cut	10381818	2
Caelo	Eleutherococcus, cut	12326703	1
Caelo	Eleutherococcus, cut	10381817	1
Caelo	Eleutherococcus, cut	12326707	1
Klenk	Eleutherococcus, cut	7011A121204	1
Klenk	Eleutherococcus, cut	7011A101206	1
Klenk	Eleutherococcus, cut	7011A110714	1
Caelo	Eleutherococcus, cut	12326701	1
Caelo	Elm bark, cut	10347204	1
Caelo	Elm bark, cut	12287902	2
Caelo	Elm bark, cut	10347203	1
Klenk	Elm bark, cut	841a120413	1
Klenk	Elm bark, cut	841A1101120	1
Aurica / 11	Equisetum stem	521302898	1
Bomba/AHD	Equisetum stem	280449	3
Bombastus	Equisetum stem	273963	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Equisetum stem	275891	3
Bombastus	Equisetum stem	264100	1
Bombastus	Equisetum stem	272552	2
Bombastus	Equisetum stem	265924	1
Bombastus	Equisetum stem	278107	1
Bombastus	Equisetum stem	18111304	1
Bombastus	Equisetum stem	6011401	1
Bombastus	Equisetum stem	280647	1
Bombastus	Equisetum stem	268321	1
Bombastus	Equisetum stem	264101	1
Bombastus	Equisetum stem	274714	1
Caelo	Equisetum stem	13344309	3
Caelo	Equisetum stem	11021901	1
Caelo	Equisetum stem	11076302	2
Caelo	Equisetum stem	3091201	1
Caelo	Equisetum stem	11076306	6
Caelo	Equisetum stem	8101201	1
Caelo	Equisetum stem	17101203	1
Caelo	Equisetum stem	20111212	1
Caelo	Equisetum stem	11076303	13
Caelo	Equisetum stem	2658181	1
Caelo	Equisetum stem	10328901	1
Caelo	Equisetum stem	1288804	1
Caelo	Equisetum stem	8041301	1
Caelo	Equisetum stem	8051302	1
Caelo	Equisetum stem	12288802	2
Caelo	Equisetum stem	6081304	1
Caelo	Equisetum stem	311042	1
Caelo	Equisetum stem	13159702	10
Caelo	Equisetum stem	13159706	5
Caelo	Equisetum stem	13091301	1
Caelo	Equisetum stem	13159704	6
Caelo	Equisetum stem	9101313	1
Caelo	Equisetum stem	30101305	1
Caelo	Equisetum stem	13344305	1
Caelo	Equisetum stem	2011408	1
Caelo	Equisetum stem	13344304	5
Caelo	Equisetum stem	13344311	1
Caelo	Equisetum stem	13350301	1
Caelo	Equisetum stem	13350309	1
Caelo	Equisetum stem	15015404	1
Caelo	Equisetum stem	10328915	1
Caelo	Equisetum stem	11021904	1
Caelo	Equisetum stem	11076307	1
Caelo	Equisetum stem	12288808	9
Caelo	Equisetum stem	282573	1
Caelo	Equisetum stem	13200201	1
Caelo	Equisetum stem	10375520	1
Caelo	Equisetum stem	13159705-3387310190	1
Caelo	Equisetum stem	13153702	1
Caelo	Equisetum stem	1359702	1
Caelo	Equisetum stem	13159705	6
Caelo	Equisetum stem	13344303	6
Caelo	Equisetum stem	12288809	3
Caelo	Equisetum stem	13159702-3464312101	1
Caelo	Equisetum stem	13344302	3
Caesar & Loretz Gm…	Equisetum stem	10375510	2
Caesar & Loretz Gm…	Equisetum stem	12288801	16
Euro OTC	Equisetum stem	3831A130610	5
Finze	Equisetum stem	11076305	8

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Galke	Equisetum stem	19663	5
Galke	Equisetum stem	22061	1
Gehe	Equisetum stem	10375515	1
Gehe	Equisetum stem	11076301	4
Gehe	Equisetum stem	12288803	14
Klenk	Equisetum stem	3831A111124	4
Hepart AG	Equisetum stem	B-695,kbA	1
Hubertus Apotheke	Equisetum stem	3831C140403	1
KBA Ware	Equisetum stem	21879	6
Klenk	Equisetum stem	3831a120611	1
Klenk	Equisetum stem	2213U01642	1
Klenk	Equisetum stem	3831A121018	6
Klenk	Equisetum stem	3831A120903	8
Klenk	Equisetum stem	3831A110922	1
Klenk	Equisetum stem	3831A120018	1
Klenk	Equisetum stem	3831A1230726	1
Klenk	Equisetum stem	3831c131104	1
Klenk	Equisetum stem	3831C131104	1
Klenk	Equisetum stem	3831A11124	1
Klenk	Equisetum stem	4713U01642	1
Klenk	Equisetum stem	3831A110601	1
Klenk	Equisetum stem	3831A120529	8
Klenk	Equisetum stem	4413Q1642	1
Klenk	Equisetum stem	3831A120611	10
Noweda	Equisetum stem	12231401	6
Klenk	Equisetum stem	3831A120726	18
Caelo	Equisetum stem	13344306	1
Caelo	Equisetum stem	12288804	11
Phönix	Equisetum stem	12288807	2
Sanacorp	Equisetum stem	13344307	1
Caelo	Equisetum stem	10375507	2
Caelo	Equisetum stem		2
Wolf	Equisetum stem	B-695	1
Wolf	Equisetum stem	B233885	4
apomix	Ergotamine tartrate	15L01-B02	1
Fagron	Ergotamine tartrate	15B16-B05-308417	1
Fagron	Ergotamine tartrate	15L01-B02-341852	1
Fagron	Ergotamine tartrate	18D05-B01-358419	2
Fagron	Ergotamine tartrate	18D05-B01-36779	1
Euro OTC	Ethyl hydrogen fumarate calcium	1510005-01	12
Lab.Offichem	Ethyl hydrogen fumarate calcium	1412007.0525	1
Lab.Offichem	Ethyl hydrogen fumarate calcium	1801004.0525	1
Lab.Offichem	Ethyl hydrogen fumarate calcium	1806023.0525	1
Fagron	Ethyl hydrogen fumarate mag…	14H27-B04-299502	6
Lab.Offichem	Ethyl hydrogen fumarate mag…	1604034.0527	1
Lab.Offichem	Ethyl hydrogen fumarate mag…	1805051.0527	1
Caelo	Eucalyptus leaf	12225203	3
Klenk	Eucalyptus leaf	2011B120419	6
Caelo	Eucalyptus leaf	9346811	1
Caelo	Eucalyptus leaf	12225202	1
Caelo	Eucalyptus leaf	122250204	1
Caelo	Eucalyptus leaf	12225206	1
Caelo	Eucalyptus leaf	11307708	2
Klenk	Eucalyptus leaf	B120419	1
Klenk	Eucalyptus leaf	B130306	2
Klenk	Eucalyptus leaf	2011B130306	4
Klenk	Eucalyptus leaf	2011b130306	1
Klenk	Eucalyptus leaf	2011B130306-35294110	1
VDL	Eucalyptus leaf	2011B110801	4
Bombastus	Euphrasy herb	274553	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Euphrasy herb	270726	2
Bombastus	Euphrasy herb	278108	2
Bombastus	Euphrasy herb	277846	1
Caelo	Euphrasy herb	112211643	1
Caelo	Euphrasy herb	11030810	1
Caelo	Euphrasy herb	29011302	1
Caelo	Euphrasy herb	12103202	9
Caelo	Euphrasy herb	12103203	10
Caelo	Euphrasy herb	7051302	1
Caelo	Euphrasy herb	312052	1
Caelo	Euphrasy herb	13180001	5
Caelo	Euphrasy herb	30101307	1
Caelo	Euphrasy herb	13180004	5
Caelo	Euphrasy herb	12103201	1
Caelo	Euphrasy herb	13180005	2
Caelo	Euphrasy herb	8011419	1
Caelo	Euphrasy herb	13180008	1
Caelo	Euphrasy herb	14019107	1
Caelo	Euphrasy herb	1213202	1
Caelo	Euphrasy herb	14019102	2
Caelo	Euphrasy herb	13180002	5
Caelo	Euphrasy herb	11030812	4
Galke	Euphrasy herb	20262	2
Klenk	Euphrasy herb	15029806	1
Klenk	Euphrasy herb	B101206	1
Klenk	Euphrasy herb	B130430	1
Klenk	Euphrasy herb	3871B130430	1
Caelo	Euphrasy herb	11030811	3

F

Supplier	Substance	Batch	Spectra
AHD	Fennel, bitter	15006502	1
AHD;11.05.15;3,23	Fennel, bitter	14376408	3
Alfred Galke	Fennel, bitter	18270	1
Bahnhof-Apotheke	Fennel, bitter	11-121029	1
Bombastus	Fennel, bitter	268130	2
Bombastus	Fennel, bitter	285609	1
Bombastus	Fennel, bitter	296877	3
Bombastus	Fennel, bitter	307641	1
Bombastus	Fennel, bitter	299386	3
Bombastus	Fennel, bitter	289870	2
Bombastus	Fennel, bitter	299385	3
Bombastus	Fennel, bitter	280891	2
Bombastus	Fennel, bitter	289870	1
Bombastus	Fennel, bitter	289869	2
Bombastus	Fennel, bitter	293627	1
Bombastus	Fennel, bitter	275922	4
Cae	Fennel, bitter	Int.Ch.314090	1
Caelo	Fennel, bitter	16061202	1
Caelo	Fennel, bitter	11185501	1
Caelo	Fennel, bitter	6091201	1
Caelo	Fennel, bitter	12094703	2
Caelo	Fennel, bitter	1209474	1
Caelo	Fennel, bitter	12035102	2
Caelo	Fennel, bitter	27121201	1
Caelo	Fennel, bitter	12167102	4
Caelo	Fennel, bitter	11016330	1
Caelo	Fennel, bitter	402311545	1
Caelo	Fennel, bitter	12094710	4
Caelo	Fennel, bitter	12094712	4

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Fennel, bitter	12094716	8
Caelo	Fennel, bitter	7031306	1
Caelo	Fennel, bitter	13020802	6
Caelo	Fennel, bitter	12094720	7
Caelo	Fennel, bitter	4061302	1
Caelo	Fennel, bitter	5061302	1
Caelo	Fennel, bitter	12094721	3
Caelo	Fennel, bitter	12094719	4
Caelo	Fennel, bitter	12094724	4
Caelo	Fennel, bitter	13200401	4
Caelo	Fennel, bitter	14111301	1
Caelo	Fennel, bitter	13148303	2
Caelo	Fennel, bitter	12362710	1
Caelo	Fennel, bitter	13148305	3
Caelo	Fennel, bitter	9121305	1
Caelo	Fennel, bitter	13200402	2
Caelo	Fennel, bitter	13148306	1
Caelo	Fennel, bitter	13371605	1
Caelo	Fennel, bitter	13371610	1
Caelo	Fennel, bitter	13371610	2
Caelo	Fennel, bitter	13398502	1
Caelo	Fennel, bitter	5121401	1
Caelo	Fennel, bitter	13398502	1
Caelo	Fennel, bitter	14376405	1
Caelo	Fennel, bitter	15006507	1
Caelo	Fennel, bitter	15443203	2
Caelo	Fennel, bitter	15443205	2
Caelo	Fennel, bitter	15443209	3
Caelo	Fennel, bitter	154443204	1
Caelo	Fennel, bitter	15443213	1
Caelo	Fennel, bitter	16298101	1
Caelo	Fennel, bitter	17341502	1
Caelo	Fennel, bitter	14255802	3
Caelo	Fennel, bitter	12167101	1
Caelo	Fennel, bitter	12094715	4
Caelo	Fennel, bitter	12345678	1
Caelo	Fennel, bitter	16005902	1
Caelo	Fennel, bitter	15007601	1
Caelo	Fennel, bitter	14376408;21S08	1
Caelo	Fennel, bitter	17341515	3
Caelo	Fennel, bitter	13148304	24
Caelo	Fennel, bitter	12094717	1
Caelo	Fennel, bitter	12035102	1
Caelo	Fennel, bitter	15443202	5
Caelo	Fennel, bitter	15443215	5
Caelo	Fennel, bitter	12094726	2
Caelo	Fennel, bitter	15141004	1
Caelo	Fennel, bitter	15443208	2
Caelo	Fennel, bitter	15443212	4
Caelo	Fennel, bitter	1302081	1
Caelo	Fennel, bitter	13020801	4
Caelo	Fennel, bitter	1320041	1
Caelo	Fennel, bitter	13148307	1
Caelo	Fennel, bitter	15006501	2
Caelo	Fennel, bitter	1S443206	1
Caelo	Fennel, bitter	14376406	2
Caelo	Fennel, bitter	15443216	2
Caelo	Fennel, bitter	19178804	2
Caelo	Fennel, bitter	14376402	1
Caelo	Fennel, bitter	15006508	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Fennel, bitter	15443204	8
Caelo	Fennel, bitter	17341503	1
Caelo	Fennel, bitter	17341510	1
Caelo	Fennel, bitter	12094716-3408310191	1
Caelo	Fennel, bitter	13148304-3500411070	1
Caelo	Fennel, bitter	14376401	2
Caelo	Fennel, bitter	16298102	1
Caesar & Loretz Gm...	Fennel, bitter	11016331	1
Caesar & Loretz Gm...	Fennel, bitter	11016319	1
Caesar & Loretz Gm...	Fennel, bitter	12094705	4
Caesar & Loretz Gm...	Fennel, bitter	12094705	2
Caesar & Loretz Gm...	Fennel, bitter	12094707	6
Caesar & Loretz Gm...	Fennel, bitter	12094711	2
Caesar & Loretz Gm...	Fennel, bitter	12094725	8
Defektur	Fennel, bitter	7/13	1
Defektur	Fennel, bitter	52/13	1
Defektur	Fennel, bitter	57/13	1
Fagron	Fennel, bitter	1406211545	1
Fagron	Fennel, bitter		1
Fagron	Fennel, bitter	6858913	1
Gahlke	Fennel, bitter	20362	1
galke	Fennel, bitter	19938	3
Galke	Fennel, bitter	22176	1
GALKE	Fennel, bitter	27755	1
Gehe	Fennel, bitter	2860A120412	24
Caelo	Fennel, bitter	1250117/15443216	1
Hepart AG	Fennel, bitter	B492,kbA	1
K	Fennel, bitter	2860A160302	1
Klenk	Fennel, bitter	2860A110704	4
Klenk	Fennel, bitter	3812A-01545	1
Klenk	Fennel, bitter	2880N120418	4
Klenk	Fennel, bitter	2860A140224	1
Klenk	Fennel, bitter	2860A140612	18
Klenk	Fennel, bitter	2860A140224	1
Klenk	Fennel, bitter	2860A130513	2
Klenk	Fennel, bitter	2860A150320	21
Klenk	Fennel, bitter	2860A140613	3
Klenk	Fennel, bitter	2866B100211	1
Klenk	Fennel, bitter	2866B130206	1
Klenk	Fennel, bitter	2866B110318	1
Klenk	Fennel, bitter	2860A160606	1
Klenk	Fennel, bitter	2860,A150617	1
Klenk	Fennel, bitter	28060A140612	1
Klenk	Fennel, bitter	2860a-140224	1
Klenk	Fennel, bitter	2860a120412	3
Kottas	Fennel, bitter	P15301479	1
Lamotte / Sanacorp	Fennel, bitter	2860A150617	6
Noweda	Fennel, bitter	2860A180212	1
Noweda 06.04.2016	Fennel, bitter	15443201	1
Caelo	Fennel, bitter	12094704	4
Phönix	Fennel, bitter	12094708	2
Caelo	Fennel, bitter	2150317	1
Klenk	Fennel, bitter	2880A100503	2
Caelo	Fennel, bitter	15006506	1
Caelo	Fennel, bitter	17020603	1
siehe Protokoll (Galke)	Fennel, bitter	sieheProtokoll	2
Spangro/gepepharm	Fennel, bitter	15007602	2
Klenk	Fennel, bitter	2860A130226	8
Wolf	Fennel, bitter	B-362	1
Wolf	Fennel, bitter	B362	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Wolf	Fennel, bitter	B-493	1
Wolf	Fennel, bitter	B-682	1
Wolf	Fennel, bitter	B382	1
Wolf	Fennel, bitter	B492	1
Wolf	Fennel, bitter	B-492	5
Caelo	Fennel, sweet	311903	1
Fagron	Fennel, sweet	2870A130304	3
Fargron/Noweda	Fennel, sweet	2870A150810	1
Klenk	Fennel, sweet	2870A140528	2
Klenk	Fennel, sweet	2870130304A	1
Klenk	Fennel, sweet	2870A131002	1
Fagron	Fentanyl citrate	17L14-B04-525660	1
Fagron	Fentanyl citrate	20100911-1	1
Fagron	Fentanyl citrate	10H20-N02	1
Fagron	Fentanyl citrate	16E26-B01-525231	1
Fagron	Fentanyl citrate	18B12-B06	1
Fagron	Fentanyl citrate	16J06-B03-525432	1
Fagron	Fentanyl citrate	18L27-B03-525914	2
Fagron	Fentanyl citrate	14Jo3-B06-525002	1
Fagron	Fentanyl citrate	14J03-B06-525002	1
Fagron	Fentanyl citrate	19D09-B04-525979	1
Fagron	Fentanyl citrate	18L27-B03-525913	1
Fagron	Fentanyl citrate	19E27-K04	1
Fagron	Fentanyl citrate	19K21-F02-526085	2
Fagron	Fentanyl citrate	19K21-F025	1
Fagron	Fentanyl citrate	20E20-F12	1
Fagron	Fentanyl citrate	17L14-B04-525639	1
Fagron	Fentanyl citrate	16E26-B01-525232	1
Fagron	Fentanyl citrate	20E20-F12-526324	1
Fagron	Fentanyl citrate	20E28-K01	1
Fagron	Fentanyl citrate	19-00252	1
Fargon/Gehe	Fentanyl citrate	21A19-K01	1
Apofit	Fenugreek	222392	1
Caelo	Fenugreek	12252601	2
Caelo	Fenugreek	11313203	1
Caelo	Fenugreek	13013801	1
Caelo	Fenugreek	1131206	1
Caelo	Fenugreek	12252603	3
Caelo	Fenugreek	13013803	6
Caelo	Fenugreek	13013805	3
Gehe	Fenugreek	11313204	1
Gehe	Fenugreek	13013811	2
Klenk	Fenugreek	7260A130603	3
Klenk	Fenugreek	9011301	1
Klenk	Fenugreek	A120118	2
Klenk	Fenugreek	8061301	1
Klenk	Fenugreek	A130603	1
Klenk	Fenugreek	7260A110530	2
Klenk	Fenugreek	7260A120118	2
Phoenix	Fenugreek	11313206	7
Caelo	Fenugreek	12252602	2
Caelo	Fenugreek, powdered	12149605	1
Caelo	Fenugreek, powdered	12149607	1
Caelo	Fenugreek, powdered	13398302	1
Caelo	Fenugreek, powdered	15308703	2
Caelo	Fenugreek, powdered	7264a110201	2
Caelo	Fenugreek, powdered	15120506	1
Caelo	Fenugreek, powdered	14057807	1
Caelo	Fenugreek, powdered	15308704	1
Caelo	Fenugreek, powdered	14377201	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Fenugreek, powdered	14057801	1
Fagron	Fenugreek, powdered	12149603	1
Ichthyol/Phoenix	Fenugreek, powdered	14377205	1
Klenk	Fenugreek, powdered	A110201	1
Klenk	Fenugreek, powdered	12082014A	1
Klenk	Fenugreek, powdered	7264A110201	9
Klenk	Fenugreek, powdered	7264B150303	1
Nachprüfung	Fenugreek, powdered	2412E02239	1
Caelo	Feverfew	12380204	1
Caelo	Feverfew	12380203	5
Sanacorp	Feverfew	12380201	2
Caelo	Flax weed herb	11104507	8
Caelo	Flax weed herb	13007502	2
Caelo	Flax weed herb	13007505	1
Caelo	Flax weed herb	14005303	1
Caelo	Flax weed herb	14005305	3
Caelo	Flax weed herb	14197204	1
Caelo	Flax weed herb	1711924	1
Caelo	Flax weed herb	16292809	1
Caelo	Flax weed herb	16292801	1
Caelo	Flax weed herb	11104505	1
Caelo	Flax weed herb	13007507	7
Klenk	Flax weed herb	4011B131115	3
Klenk	Flax weed herb	4011B121207	2
Bombastus	Frangula bark	268407	1
Bombastus	Frangula bark	270733	1
Bombastus	Frangula bark	273926	1
Bombastus	Frangula bark	275998	2
Bombastus	Frangula bark	281284	2
Bombastus	Frangula bark	278599	3
Bombastus	Frangula bark	238812	1
Caelo	Frangula bark	11254001	2
Caelo	Frangula bark	11340801	1
Caelo	Frangula bark	12185901	10
Caelo	Frangula bark	10061301	1
Caelo	Frangula bark	12186006	8
Caelo	Frangula bark	13203008	1
Caelo	Frangula bark	6011402	1
Caelo	Frangula bark	14163102	1
Caelo	Frangula bark	eztetdt	1
Caelo	Frangula bark	12186001	1
Caelo	Frangula bark	12186003	1
Caelo	Frangula bark	12186005	1
Caelo	Frangula bark	1286003	1
Caelo	Frangula bark	12186002	16
Caelo	Frangula bark	121860006	1
Caesar&loretz,Phoenix	Frangula bark	14163104	1
Finze	Frangula bark	249091	1
Gehe	Frangula bark	11254003	2
Gehe	Frangula bark	11254004	4
Gehe	Frangula bark	11254006	4
Klenk	Frangula bark	661B110412	4
Klenk	Frangula bark	6621B110412	1
Klenk	Frangula bark	661B130306	1
Klenk	Frangula bark	661B-090903	1
Klenk	Frangula bark	661B-110412	1
Caelo	Frangula bark	12186004	11
Caelo	Frankincense	12120005	5
Caelo	Frankincense	10349210	1
Caelo	Frankincense	10349213	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Frankincense	12120008	2
Caelo	Frankincense	13112801	5
Caelo	Frankincense	13112809	2
Caelo	Frankincense	4614M-02030	1
Caelo	Frankincense	15140810	1
Caelo	Frankincense	802929	1
Caelo	Frankincense	15140809	2
Caelo	Frankincense	15140805	2
Caelo	Frankincense	15140804	1
Caelo	Frankincense	12120006	3
Caelo	Frankincense	13112803	1
Caelo	Frankincense	13112807	1
Caelo	Frankincense	14107803	2
Caelo	Frankincense	12120012-3421310191	1
Caelo	Frankincense	13112803-3494411030	1
Fagron	Frankincense		1
Gahlke	Frankincense	21949	1
vedono	Frankincense	12120009	5
vedono	Frankincense	12120012	1
Euro OTC	Frankincense extract 80%	1104005V-04	2
Euro OTC	Frankincense extract 80%	1705033-01	1
Klenk	Fraxinella root, cut	6271B140708	1
Fagron	Fuchsine	12A03-N06	1
Fagron	Fuchsine	12F28-N02	1
Fagron	Fuchsine	12G18-N01	1
Fagron	Fuchsine	13H23-M04	2
Fagron	Fuchsine	13A30-N05	1
Caelo	Fumitory	11101406	1
Caelo	Fumitory	11101410	1
Caelo	Fumitory	11101411	3
Caelo	Fumitory	11101413	3
Caelo	Fumitory	31081201	1
Caelo	Fumitory	7111201	1
Caelo	Fumitory	13202902	11
Caelo	Fumitory	13202905	2
Caelo	Fumitory	12103408	5
Caelo	Fumitory	12103405	7
Caelo	Fumitory	11101408	1
Caelo	Fumitory	12103404	2
Caelo	Fumitory	12103407	6
Caelo	Fumitory	1320902	1
Caelo	Fumitory	72878477	1
Caelo	Fumitory	8312901	1
Gehe	Fumitory	12103402	2
Kenk / Phoenix	Fumitory	3881B111013	2
Klenk	Fumitory	B120410	1
Klenk	Fumitory	3881B100127	1

G

Supplier	Substance	Batch	Spectra
Caelo	Galangal root	12330305	1
Caelo	Galangal root	11375904	1
Caelo	Galangal root	12330306	2
Caelo	Galangal root	15128008	1
Caelo	Galangal root	16196901	1
Caelo	Galangal root	4056371	1
Caelo	Galangal root	94614429	1
Caelo	Galangal root	16196904	1
Caelo	Galangal root	12125004	2
Caelo	Galangal root	1215004	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Galangal root	12330303	1
Caelo	Galangal root	15045701	1
Gehe	Galeopsis herb, cut	3911A130320	6
Klenk	Galeopsis herb, cut	3911A080409	1
Klenk	Galeopsis herb, cut	3911A130110	3
Klenk	Galeopsis herb, cut	3911A090219	2
Klenk	Galeopsis herb, cut	3911a130320	1
Caelo	Garden violet, cut	11124008	1
Caelo	Garden violet, cut	13038701	4
Caelo	Garden violet, cut	11124007	1
Caelo	Garden violet, cut	1303872	1
Caelo	Garden violet, cut	13038703	2
Caelo	Garden violet, cut	10011403	1
Caelo	Garden violet, cut	13232107	1
Caelo	Garden violet, cut	11124007-3284310662	1
an	Gentian root	6311b130305	1
Anzag EK7,91 08.08.12	Gentian root	10263407	1
Caelo	Gentian root	10263404	1
Caelo	Gentian root	10263411	1
Caelo	Gentian root	30011301	1
Caelo	Gentian root	19071304	1
Caelo	Gentian root	Int.Ch:313091	1
Caelo	Gentian root	12244608	1
Caelo	Gentian root	6311B130305	2
Caelo	Gentian root	13156102	1
Caelo	Gentian root	12244607	1
Caesar & Loretz Gm…	Gentian root	12244603	2
Galke	Gentian root	19192	2
Klenk	Gentian root	6311B130205	2
Klenk	Gentian root	6311B140704	1
Klenk	Gentian root	6311A120723	3
Klenk	Gentian root	6311a120723	2
Klenk	Gentian root	1911E-02142	1
kräuter schulte	Gentian root	52348	1
Phoenix	Gentian root	6311B120104	1
Phönix	Gentian root	269197	2
Phönix	Gentian root	6311B120315	8
Richter	Gentian root	P200907	1
-	Gentian root, powdered	130063	1
Caelo	Gentian root, powdered	15011403	1
Caelo	Gentian root, powdered	14215601	1
Caelo	Gentian root, powdered	12007106	1
Galke	Geum urbanum herb, cut	20881	1
Kräuter Schulte	Geum urbanum herb, cut	51737	1
Caelo	Ginger	11325715	2
Caelo	Ginger	11325716	1
Caelo	Ginger	19121201	1
Caelo	Ginger	11325719	3
Caelo	Ginger	13100602	2
Caelo	Ginger	13310604	4
Caelo	Ginger	12180604	1
Caelo	Ginger	13100604	1
Caelo	Ginger	11325703	2
Caelo	Ginger	11325712	1
Caelo	Ginger	13100605	4
Caelo	Ginger	13310602	2
Caelo	Ginger	12164911-3368319002	1
Galke	Ginger	20633	1
Galke	Ginger	21766	2
Klenk	Ginger	6951B110119	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Ginger	6951B110822	1
Klenk	Ginger	6951B100302	1
Klenk	Ginger	6951B130110	1
Phönix	Ginger	13310601	1
Richter	Ginger	KR27992	1
Caelo	Ginger, peeled, powdered	12164901	1
Caelo	Ginger, peeled, powdered	13092013B	1
Caelo	Ginger, peeled, powdered	12164911	1
Klenk	Ginger, peeled, powdered	6954B16029	1
Klenk	Ginger, peeled, powdered	6954B170127	1
Klenk	Ginger, peeled, powdered	6954B110801	1
Klenk	Ginger, peeled, powdered	B121030	2
Klenk	Ginger, peeled, powdered	6954B130418	2
Klenk	Ginger, peeled, powdered	6954B121030	2
Klenk	Ginger, peeled, powdered	6954B160429	5
Klenk	Ginger, peeled, powdered	KS200260	1
Klenk	Ginger, peeled, powdered	6954B160929	2
Caelo	Ginkgo leaf	12151709	2
Caelo	Ginkgo leaf	15077407	1
Caelo	Ginkgo leaf	13340907	1
Caelo	Ginkgo leaf	13340904	1
Caelo	Ginkgo leaf	13340906	1
Caelo	Ginkgo leaf	12373604	1
Caelo	Ginkgo leaf	15077410	1
Nachprüfung	Ginkgo leaf	2461A100429	11
Bombastus	Ginseng root	13150903	1
Caelo	Ginseng root	13341001	1
Caelo	Ginseng root	12080218	1
Caelo	Goat's rue, cut	11307903	1
Caelo	Goat's rue, cut	11175104	1
Caelo	Goat's rue, cut	11307901	1
Caelo	Goat's rue, cut	12017907	3
Caelo	Goat's rue, cut	12017914	1
Caelo	Goat's rue, cut	12017913	2
Caelo	Goat's rue, cut	12343303	6
Caelo	Goat's rue, cut	12343302	4
Caelo	Goat's rue, cut	5122013e	1
Caelo	Goat's rue, cut	12343305	3
Caelo	Goat's rue, cut	12343308	1
Galke	Goat's rue, cut	8378	2
Klenk	Goat's rue, cut	3901C110905	1
Klenk	Goat's rue, cut	3901B140801	1
Caelo	Goat's rue, cut	12017912	1
Sanacorp	Goat's rue, cut	12017911	1
Caelo	Goldenrod	12343103	17
Anzag 17.04.13 ek:…	Goldenrod	4521A110816	2
Aurica	Goldenrod	521201267	1
Aurica	Goldenrod	224133	1
Bomba/AHD	Goldenrod	279526	1
Bombastus	Goldenrod	261756	1
Bombastus	Goldenrod	271459	1
Bombastus	Goldenrod	270047	2
Bombastus	Goldenrod	271460	1
Bombastus	Goldenrod	278697	2
Bombastus	Goldenrod	209974	1
Caelo	Goldenrod	314050-1-p	1
Caelo	Goldenrod	11207010	3
Caelo	Goldenrod	15061203	1
Caelo	Goldenrod	265283	1
Caelo	Goldenrod	11280301	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Goldenrod	17091203	1
Caelo	Goldenrod	11280308	9
Caelo	Goldenrod	20111209	1
Caelo	Goldenrod	112080308	1
Caelo	Goldenrod	12319002	2
Caelo	Goldenrod	28051302	1
Caelo	Goldenrod	6081302	1
Caelo	Goldenrod	12343104	5
Caelo	Goldenrod	4091302	1
Caelo	Goldenrod	12343102	3
Caelo	Goldenrod	14112012	1
Caelo	Goldenrod	27121302	1
Caelo	Goldenrod	4021405	1
Caelo	Goldenrod	12343109	1
Caelo	Goldenrod	13386903	1
Caelo	Goldenrod	13386901	1
Caelo	Goldenrod	14018404	1
Caelo	Goldenrod	2656153	1
Caelo	Goldenrod	12343105	1
Caelo	Goldenrod	11280309	1
Caelo	Goldenrod	12336801	1
Caelo	Goldenrod	12319007	21
Caelo	Goldenrod	12319006	3
Caelo	Goldenrod	12319004	10
Caelo	Goldenrod	4113A-01684	1
Caelo	Goldenrod	11280310	6
Caelo	Goldenrod	12343106	1
Caesar & Loretz Gm…	Goldenrod	11207014	3
Galke	Goldenrod	21079	2
Gehe	Goldenrod	11207011	1
Gehe	Goldenrod	11280311	2
Caelo	Goldenrod	12343101	3
Klenk	Goldenrod	A110209	1
Klenk	Goldenrod	4521A-110816	1
Klenk	Goldenrod	4521A100414	1
Klenk	Goldenrod	4521A110209	4
Noweda	Goldenrod	11280306	3
Caelo	Goldenrod	12319003	22
Bombastus	Goldenrod	274290	1
Caelo	Goldenrot, European	13386908	1
Caelo	Goldenrot, European	12343102	1
Caelo	Goldenrot, European	12343103-3466312121	1
Klenk	Goldenrot, European	1781B110706	1
Kenk / Phoenix	Goldenrot, European	1781B110826	1
Sanacorp	Goldenrot, European	12343103	1
-	Greater celandine herb	810I-01632	1
Klenk	Greater celandine herb	1406111632	1
Caelo	Greater celandine herb	311092	1
Galke	Greater celandine herb	20937	3
Klenk	Greater celandine herb	3731A110301	6
Klenk	Greater celandine herb	3731A120611	4
Klenk	Greater celandine herb	4711E-01632	1
Klenk	Greater celandine herb	3731A130904	5
Klenk	Greater celandine herb	3731B100205	1
Klenk	Greater celandine herb	3731K120904	4
Caelo	Ground ivy herb	11052315	1
Caelo	Ground ivy herb	11052314	1
Caelo	Ground ivy herb	11374611	2
Caelo	Ground ivy herb	11374615	1
Caelo	Ground ivy herb	11374606	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ground ivy herb	11374602	1
Caelo	Ground ivy herb	11374609	1
Caelo	Ground ivy herb	11052318	2
Gutenberg-Apotheke	Ground ivy herb	11374610	3
Klenk	Ground ivy herb	3991B110304	1
Klenk	Ground ivy herb	3991B130502	2
Phönix	Ground ivy herb	11374608	1
Richter	Ground ivy herb	s99/09	1
Caelo	Guaiacum wood	11352001	1
Caelo	Guaiacum wood	4011M-01778	1
Caelo	Guaiacum wood	11352008	1
Caelo	Guaiacum wood	8041401	1
Caelo	Guaiacum wood	16136708	1
Caelo	Guaiacum wood	10353102	1
Caelo	Guaiacum wood	11352010	1
Caelo	Guaiacum wood	14008203	1
Caelo	Guaiacum wood	16136710	1
Caelo	Guaiacum wood	16136706	1
Caelo	Guaiacum wood	16136705	1
Caelo	Guaiacum wood	11352012	1
sana 09.12.14 3,75	Guaiacum wood	13343802	1

H

Supplier	Substance	Batch	Spectra
Caelo	Hamamelis bark, cut	12361301	1
Caelo	Hamamelis bark, cut	13123701	1
Caelo	Hamamelis bark, cut	13123703	1
Caelo	Hamamelis leaf	10102915	1
Caelo	Hamamelis leaf	12165805	1
Caelo	Hamamelis leaf	12164802	1
Caelo	Hamamelis leaf	14356103	1
Caelo	Hamamelis leaf	30287394	1
Caelo	Hamamelis leaf	13269904	1
Caelo	Hamamelis leaf	13269902	2
Caelo	Hamamelis leaf	12164804	1
Euro OTC	Hamamelis leaf	12164805	1
Klenk	Hamamelis leaf	B110214	1
Klenk	Hamamelis leaf	2051B110214	1
Caelo	Hamamelis leaf	13269905	1
Alliance	Hawthorn flower	13010403	1
Caelo	Hawthorn flower	13010403	5
Caelo	Hawthorn flower	7121201	1
Caelo	Hawthorn flower	11068208	1
Caelo	Hawthorn flower	11068206	1
Caelo	Hawthorn flower	13010402	2
Caelo	Hawthorn flower	11068209	1
Caelo	Hawthorn flower	13010402	3
Caelo	Hawthorn flower	11068202	1
Caelo	Hawthorn flower	21051301	1
Caelo	Hawthorn flower	25101301	1
Caelo	Hawthorn flower	13253303	1
Caelo	Hawthorn flower	13253304	1
Caelo	Hawthorn flower	1351B130819	3
Caesar & Loretz GmbH	Hawthorn flower	11068206	3
Hepart AG	Hawthorn flower	13010401	1
Klenk	Hawthorn flower	1351B111207	4
Klenk	Hawthorn flower	B1112107	1
Caelo	Hawthorn fruit	11278202	1
Caelo	Hawthorn fruit	12326308	1
Caelo	Hawthorn fruit	13101402	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hawthorn fruit	12326306	1
Caelo	Hawthorn fruit	13367203	1
Caelo	Hawthorn fruit	12326307	2
Klenk	Hawthorn fruit	2806B110818	2
Klenk	Hawthorn fruit	2806B121203	2
Caelo	Hawthorn fruit	12326304	1
an	Hawthorn leaf with flower	1971A130930	2
Bahnhof-Apotheke	Hawthorn leaf with flower	7-121011	1
Bombastus	Hawthorn leaf with flower	264044	1
Bombastus	Hawthorn leaf with flower	267551	1
Bombastus	Hawthorn leaf with flower	272881	1
Bombastus	Hawthorn leaf with flower	267000	1
Bombastus	Hawthorn leaf with flower	273287	1
Bombastus	Hawthorn leaf with flower	278756	1
Caelo	Hawthorn leaf with flower	10273512	2
Caelo	Hawthorn leaf with flower	10273515	6
Caelo	Hawthorn leaf with flower	11366001	1
Caelo	Hawthorn leaf with flower	11068206	1
Caelo	Hawthorn leaf with flower	12225104	12
Caelo	Hawthorn leaf with flower	1222514	1
Caelo	Hawthorn leaf with flower	12225108	7
Caelo	Hawthorn leaf with flower	IntCh:313082	1
Caelo	Hawthorn leaf with flower	12225107	5
Caelo	Hawthorn leaf with flower	13276703	3
Caelo	Hawthorn leaf with flower	15188802	1
Caelo	Hawthorn leaf with flower	1518802	1
Caelo	Hawthorn leaf with flower	16025802	1
Caelo	Hawthorn leaf with flower	2225104	1
Caelo	Hawthorn leaf with flower	109076	1
Caelo	Hawthorn leaf with flower	1225107	1
Caelo	Hawthorn leaf with flower	12225207	1
Caelo	Hawthorn leaf with flower	52467476	1
Caelo	Hawthorn leaf with flower	1221707	1
Galke	Hawthorn leaf with flower	21126	3
Gehe	Hawthorn leaf with flower	1351B111207	2
Kenk / Phoenix	Hawthorn leaf with flower	1971A130307	6
Klenk	Hawthorn leaf with flower	1971A110620	5
Klenk	Hawthorn leaf with flower	1971A120215	3
Klenk	Hawthorn leaf with flower	14101301	1
Klenk	Hawthorn leaf with flower	28101307	1
Klenk	Hawthorn leaf with flower	20121302	1
Klenk	Hawthorn leaf with flower	A130307	1
Klenk	Hawthorn leaf with flower	1971a120813	2
Klenk	Hawthorn leaf with flower	1972A120727	1
Klenk	Hawthorn leaf with flower	1971A120813	20
Klenk	Hawthorn leaf with flower	1971A120727	13
Klenk	Hawthorn leaf with flower	1971a120215	1
Klenk	Hawthorn leaf with flower	1971A120813-34103101	1
Klenk	Hawthorn leaf with flower	1971A130307-3447	1
Klenk	Hawthorn leaf with flower	1971A130307-35014110	1
Bombastus	Hawthorn leaf with flower	275310	2
vedono	Hawthorn leaf with flower	12225103	4
Bahnhof-Apotheke	Hay flowers	13-121105	1
Caelo	Hay flowers	11099912	1
Caelo	Hay flowers	25101202	1
Caelo	Hay flowers	11099914	1
Caelo	Hay flowers	11099916	1
Caelo	Hay flowers	11099909	1
Caelo	Hay flowers	12317102	3
Caelo	Hay flowers	1231702	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hay flowers	12317108	3
Caelo	Hay flowers	12317107	14
Caelo	Hay flowers	13097302	9
Caelo	Hay flowers	12317110	2
Caelo	Hay flowers	13099205	1
Caelo	Hay flowers	14121301	1
Caelo	Hay flowers	13097301	1
Caelo	Hay flowers	11099902	1
Caelo	Hay flowers	12317104	10
Caelo	Hay flowers	3713E-01459	1
Caelo	Hay flowers	3713F-01459	1
Caelo	Hay flowers	12317101	8
Caelo	Hay flowers	12371707	1
Galke	Hay flowers	21926	1
Klenk	Hay flowers	A130304	1
Klenk	Hay flowers	10192103	1
Klenk	Hay flowers	1400A120116	1
Nachprüfung	Hay flowers	1911E01459	1
Caelo	Hay flowers	11099915	1
Caelo	Heather flower, rubbed	10270516	1
Caelo	Heather flower, rubbed	13014204	5
Caelo	Heather flower, rubbed	13014206	1
Klenk	Heather flower, rubbed	13014202	1
Alliance	Heather, cut	255389	1
Bombastus	Heather, cut	278314	1
Caelo	Heather, cut	28061201	1
Caelo	Heather, cut	9291512	1
Caelo	Heather, cut	19111203	1
Caelo	Heather, cut	11011209	3
Caelo	Heather, cut	11102901	1
Caelo	Heather, cut	13367502	1
Caesar/Noweda	Heather, cut	4911I-03224	1
Nachprüfung	Heather, cut	5110A03224	1
Caelo	Henna powder	12122301	2
Caelo	Henna powder	12122310	3
Caelo	Henna powder	13262803	2
Caelo	Henna powder	12267311	1
Klenk	Henna powder	20747A111004	1
Klenk	Henna powder	2074A111004	1
Caelo	Hop strobile	13123802	9
Bombaltus	Hop strobile	274724	1
Bombastus	Hop strobile	276976	1
Bombastus	Hop strobile	271870	1
Bombastus	Hop strobile	208502	1
Caelo	Hop strobile	15061211	1
Caelo	Hop strobile	12008307	2
Caelo	Hop strobile	1451b120817	1
Caelo	Hop strobile	5021306	1
Caelo	Hop strobile	12008317	6
Caelo	Hop strobile	12380101	6
Caelo	Hop strobile	12380103	2
Caelo	Hop strobile	1451B130107	6
Caelo	Hop strobile	6091303	1
Caelo	Hop strobile	13123803	9
Caelo	Hop strobile	12221807	1
Caelo	Hop strobile	13123902	1
Caelo	Hop strobile	4111304	1
Caelo	Hop strobile	13123807	1
Caelo	Hop strobile	30121301	1
Caelo	Hop strobile	13123803	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hop strobile	13123804	3
Caelo	Hop strobile	131223805	1
Caelo	Hop strobile	14068007	1
Caelo	Hop strobile	12221804	1
Caelo	Hop strobile	12008302	1
Caelo	Hop strobile	12008315	1
Caelo	Hop strobile	4756769	1
Caelo	Hop strobile	12008309	3
Caelo	Hop strobile	10240308	1
Caelo	Hop strobile	13187602	1
Caelo	Hop strobile	12008305	1
Caelo	Hop strobile	120008312	1
Caelo	Hop strobile	12221805	3
Caelo	Hop strobile	12221802	2
Caelo	Hop strobile	12092001	2
Caelo	Hop strobile	12008310	3
Caelo	Hop strobile	12008310	3
Caelo	Hop strobile	12006305	1
Caelo	Hop strobile	12008313	2
Caelo	Hop strobile	12008317	1
Caelo	Hop strobile	13123803-3505411011	1
Caelo	Hop strobile	13123804-3563412081	1
Galke	Hop strobile	20928	3
Galke	Hop strobile	20928	2
Galke	Hop strobile	23363	1
Caelo	Hop strobile	13123806	1
Klenk	Hop strobile	1451B120202	6
Klenk	Hop strobile	1451B111004	1
Klenk	Hop strobile	20071301	1
Klenk	Hop strobile	B130409	1
Klenk	Hop strobile	1451b130409	1
Klenk	Hop strobile	1451B140408	1
Klenk	Hop strobile	1450A110712	1
Klenk	Hop strobile	1451B130409	1
Klenk	Hop strobile	1451b130107	1
Klenk	Hop strobile	1451B130409	9
Klenk	Hop strobile	1451B-120817	1
Klenk	Hop strobile	1451B120817	7
Noweda	Hop strobile	274725	1
Caelo	Hop strobile	13123802	3
Galke	Horse chestnut flower, cut	2614	1
Klenk	Horse chestnut flower, cut	1440A110311	3
Richter	Horse chestnut flower, cut	s-09/09	1
Anzag ek:2,50EUR 15.09.12	Horse chestnut leaf	2551B111013	7
Apotheke Bühlau	Horse chestnut leaf	100416	1
Caelo	Horse chestnut leaf	11063503	2
Gehe	Horse chestnut leaf	2551B131024	1
Klenk	Horse chestnut leaf	255100903	1
Klenk	Horse chestnut leaf	N130124	2
Klenk	Horse chestnut leaf	2551N130124	3
Klenk	Horse chestnut leaf	2551B081223	1
Fagron	Hydrocortisone butyrate	16j21-b01	1
Fagron	Hydrocortisone butyrate	15G08-B16-314883	1
	Hydromorphone hydrochloride	21002482008	1
Caelo	Hydromorphone hydrochloride	15393604	1
Caelo	Hydromorphone hydrochloride	14210405	1
Caelo	Hydromorphone hydrochloride	18316002	2
Caelo	Hydromorphone hydrochloride	16123805	3
Caelo	Hydromorphone hydrochloride	16273607	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Hydromorphone hydrochloride	18188403	1
Caelo	Hydromorphone hydrochloride	1623604	1
Caelo	Hydromorphone hydrochloride	16273606	1
Caelo	Hydromorphone hydrochloride	16273602	1
Caelo	Hydromorphone hydrochloride	16273604	2
Caelo	Hydromorphone hydrochloride	18188402	2
Caelo	Hydromorphone hydrochloride	21002482004	3
Caesar & Loretz GmbH	Hydromorphone hydrochloride	18316005	3
Caesar & Loretz GmbH	Hydromorphone hydrochloride	20004514004	2
Caesar & Loretz GmbH	Hydromorphone hydrochloride	21002482001	8
Caesar & Loretz GmbH	Hydromorphone hydrochloride	20004514008	1
Caesar & Loretz Gm...	Hydromorphone hydrochloride	20004525001	4
Caesar & Loretz Gm...	Hydromorphone hydrochloride	20004514001	14
Caesar & Loretz Gm...	Hydromorphone hydrochloride	20004514009	3
Fagron	Hydromorphone hydrochloride	13I27-N05	1
Fagron	Hydromorphone hydrochloride	17F0-B01-337510	2
Fagron	Hydromorphone hydrochloride	18I27-B01-364198	1
Fagron	Hydromorphone hydrochloride	18I27-B01	1
Fagron	Hydromorphone hydrochloride	21F03-F01-379168	1
Fagron	Hydromorphone hydrochloride	15L08-B08	1
Fagron	Hydromorphone hydrochloride	17F01-B01-337510	1
Fargon - Phoenix	Hydromorphone hydrochloride	17F01-B01-3375510	1
Caelo	Hydromorphone hydrochloride	15393605	1
Fagron	Hydromorphone hydrochloride	15L08-B08-316877	1
Phönix	Hydromorphone hydrochloride	13E16-No2	1
Fagron	Hydromorphone hydrochloride	12G05-N02	1
Caelo	Hyssop herb, cut	11374304	1
Caelo	Hyssop herb, cut	13143902	1
Caesar & Loretz/ Noweda	Hyssop herb, cut	11374301	1
Galke	Hyssop herb, cut	20939	1
Phönix	Hyssop herb, cut	11374306	1
Sanacorp	Hyssop herb, cut	11374303	2
Sanacorp	Hyssop herb, cut	13336101	7

I

Supplier	Substance	Batch	Spectra
-	Iceland moss	4711E-01774	1
Anzag ek: 15,60 20...	Iceland moss	11101605	1
Bombastus	Iceland moss	13357802	1
Caelo	Iceland moss	13350805	4
Caelo	Iceland moss	11101601	1
Caelo	Iceland moss	11101607	8
Caelo	Iceland moss	12197002	1
Caelo	Iceland moss	4912E-01774	1
Caelo	Iceland moss	12187002	1
Caelo	Iceland moss	11053916	1
Caelo	Iceland moss	12187103	1
Caelo	Iceland moss	12187106	3
Caelo	Iceland moss	12187109	4
Caelo	Iceland moss	12187107	1
Caelo	Iceland moss	13350803	4
Caelo	Iceland moss	12382806	1
Caelo	Iceland moss	13350807	4
Caelo	Iceland moss	14304402	1
Caelo	Iceland moss	14304401	1
Caelo	Iceland moss	14304407	2
Caelo	Iceland moss	15297601	1
Caelo	Iceland moss	711906	1
Caelo	Iceland moss	15297606	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Iceland moss	18078207	1
Caelo	Iceland moss	12187102	21
Caelo	Iceland moss	12187108	4
Caelo	Iceland moss	15297605	4
Caelo	Iceland moss	14304403	2
Caelo	Iceland moss	11053911	1
Caelo	Iceland moss	1287102	1
Caelo	Iceland moss	14304409	6
Caelo	Iceland moss	9052804	2
Caelo	Iceland moss	15297603	1
caesar&loretz,Phönix	Iceland moss	14304404	3
Galke	Iceland moss	12369	1
Gehe	Iceland moss	11101603	1
Gehe	Iceland moss	11053915	1
Gehe	Iceland moss	18079703	1
Klenk	Iceland moss	5191N110609	1
Klenk	Iceland moss	5191A140828	2
noweda	Iceland moss		1
Phönix	Iceland moss	12187104	3
Fagron	Indigo carmine	12K06-N11	1
Fagron	Indigo carmine	12A20-N067-16	1
Fagron	Indigo carmine	5132316	1
Fagron	Indigo carmine	13K12-N01	1
Fagron	Indigo carmine	11F09-N06	1
Caelo	Iron(III) sulfate hydrate	12175908	1
Caelo	Iron(III) sulfate hydrate	1512210007	1
Caelo	Iron(III) sulfate hydrate	10354412	1
Caelo	Iron(III) sulfate hydrate	12175906	1
Caelo	Iron(III) sulfate hydrate	10354404	1
Caelo	Iron(III) sulfate hydrate	10354415	1
Anzag	Ispaghula seed	11185818	1
Caelo	Ispaghula seed	4121201	1
Caelo	Ispaghula seed	4121202	1
Caelo	Ispaghula seed	9011302	1
Caelo	Ispaghula seed	10011303	1
Caelo	Ispaghula seed	413E-03369	1
Caelo	Ispaghula seed	3051302	1
Caelo	Ispaghula seed	19061308	1
Caelo	Ispaghula seed	18071301	1
Caelo	Ispaghula seed	5091319	1
Caelo	Ispaghula seed	30101302	1
Caelo	Ispaghula seed	16121302	1
Caelo	Ispaghula seed	26011401	1
Caelo	Ispaghula seed	14031408	1
Caelo	Ispaghula seed	11061405	1
Caelo	Ispaghula seed	4114001	1
Caelo	Ispaghula seed	12276527	1
Caelo	Ispaghula seed	23011505	1
Caelo	Ispaghula seed	14246602	3
Caelo	Ispaghula seed	142660	1
Caelo	Ispaghula seed	29061510	1
Caelo	Ispaghula seed	15081503	1
Caelo	Ispaghula seed	15121901	1
Caelo	Ispaghula seed	8041702	1
Caelo	Ispaghula seed	28111703	1
Caelo	Ispaghula seed	18061804	1
Caelo	Ispaghula seed	15249315	1
Caelo	Ispaghula seed	12252709	1
Caelo	Ispaghula seed	1227506	1
Caelo	Ispaghula seed	12276511	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ispaghula seed	15249319	2
Caelo	Ispaghula seed	12276501	2
Caesar/Noweda	Ispaghula seed	12276503	1
Caesar/Noweda	Ispaghula seed	12276509	3
Caesar/Noweda	Ispaghula seed	12276516	1
Cealo	Ispaghula seed	12276502	4
Klenk	Ispaghula seed	7560A130710	1
Klenk	Ispaghula seed	7560A120828	7
Klenk	Ispaghula seed	20071302	1
Klenk	Ispaghula seed	7560A130418	2
Klenk	Ispaghula seed	7560A160229	1
Klenk	Ispaghula seed	7560A140203	1
Klenk	Ispaghula seed	7560A150420	3
Caelo	Ispaghula seed	11185811	2
Caelo	Ivy leaf, cut	23121303	1
Caelo	Ivy leaf, cut	23121305	1
Caelo	Ivy leaf, cut	8061205	1
Caelo	Ivy leaf, cut	11101205	1
Caelo	Ivy leaf, cut	15101203	1
Caelo	Ivy leaf, cut	20111211	1
Caelo	Ivy leaf, cut	4011301	1
Caelo	Ivy leaf, cut	11229505	5
Caelo	Ivy leaf, cut	2031301	1
Caelo	Ivy leaf, cut	12225603	2
Caelo	Ivy leaf, cut	11041303	1
Caelo	Ivy leaf, cut	12225602	1
Caelo	Ivy leaf, cut	27111301	1
Caelo	Ivy leaf, cut	10011401	1
Caesar & Loretz/ Noweda	Ivy leaf, cut	12225606	5
Gehe	Ivy leaf, cut	2061B080402	1
Klenk	Ivy leaf, cut	B130118	1
Phönix	Ivy leaf, cut	11101102	1
Caelo	Ivy leaf, cut	12225605	5

J

Supplier	Substance	Batch	Spectra
Caelo	Jasmine flower	12143203	3
Klenk	Jasmine flower	1460A110505	1
Phönix	Jasmine flower	12143206	1
Caelo	Java tea	20111207	1
Caelo	Java tea	31121203	1
Caelo	Java tea	2221B121112	16
Caelo	Java tea	12225702	1
Caelo	Java tea	21061304	1
Caelo	Java tea	28101305	1
Caelo	Java tea	12225704	3
Caelo	Java tea	13258804	3
Caelo	Java tea	2221A110825	2
Caelo	Java tea	11212901	1
Klenk	Java tea	2221B12112	1
Klenk	Java tea	2221B110718	6
Klenk	Java tea	B110718	1
Klenk	Java tea	B121112	3
Klenk	Java tea	17121304	1
Caelo	Java tea	13258802	2
VDL	Java tea	2221B101213	1
Aurica / 11	Juniper berry	521301390	1
Aurica/Phönix	Juniper berry	521006043	1
Caelo	Juniper berry	12028610	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Juniper berry	12330505	2
Klenk	Juniper berry	2890A101201	5
Klenk	Juniper berry	2890A120709	14
Klenk	Juniper berry	A120709	3
Klenk	Juniper berry	2890a101201	3
Klenk	Juniper berry	2890a120709	1
Klenk	Juniper berry	2890A130513	2
Phoenix	Juniper berry		1
Phönix	Juniper berry	13020903	1
Sanacorp	Juniper berry	12330509	1
Caelo	Juniper berry, pounded	13031302	1
Caelo	Juniper berry, pounded	14149502	1
Caelo	Juniper berry, pounded	13367302	1
Gehe	Juniper berry, pounded	13020903	1
Gehe am 27.03.2014	Juniper berry, pounded	2890A130513	1
Klenk	Juniper berry, pounded	2896B121016	7

K

Supplier	Substance	Batch	Spectra
Caelo	Kaolin, heavy	11041610	1
Caelo	Kaolin, heavy	11350106	2
Caelo	Kaolin, heavy	11350115	1
Caelo	Kaolin, heavy	10176518	1
Caelo	Kaolin, heavy	11350124	4
Caelo	Kaolin, heavy	11350107	1
Caelo	Kaolin, heavy	82043269	1
Caelo	Kaolin, heavy	13041803	1
Caelo	Kaolin, heavy	13041835	2
Caelo	Kaolin, heavy	13041801	2
Caelo	Kaolin, heavy	13041834	1
Caelo	Kaolin, heavy	11350107	5
Caelo	Kaolin, heavy	13041803	1
Caelo	Kaolin, heavy	11350125	4
Caelo	Kaolin, heavy	13041835	1
Caelo	Kaolin, heavy	63033516	1
Klenk	Kaolin, heavy	424A100819	2
Klenk	Kaolin, heavy	45131I01190	1
Klenk	Kaolin, heavy	424A130507	4
Klenk	Kaolin, heavy	424A130507	2
Caelo	Kap-Aloe	12232102	1
Caelo	Kap-Aloe	505125	1
Caelo	Kap-Aloe	12338206	2
Caelo	Kap-Aloe	25111303	1
Caelo	Kap-Aloe	12338209	1
Caelo	Kap-Aloe	11041402	1
Caelo	Kap-Aloe	11061406	1
Caelo	Kap-Aloe	25071402	1
Caelo	Kap-Aloe	15283006	1
Caelo	Kap-Aloe	16202404	2
Caelo	Kap-Aloe	16202407	1
Caelo	Kap-Aloe	16202403	1
Caelo	Kap-Aloe	15283001	1
Caelo	Kap-Aloe	12338201	4
Caelo	Kap-Aloe	15283010	2
Caelo	Kap-Aloe	16202401	2
Caelo	Kap-Aloe	12338203	4
Caesar/Noweda	Kap-Aloe	2013E-01089	1
Caesar/Noweda	Kap-Aloe	12338211	1
Gehe	Kap-Aloe	18235801	1
phönix	Kap-Aloe	15283011	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Kap-Aloe	15283007	1
Caelo	Kap-Aloe	16202406	2
Caelo	Kelp, cut	11351109	1
Caelo	Kelp, cut	14071502	1
Caelo	Kelp, cut	11352209	1
Klenk	Kelp, cut	1051A110920	1
Caelo	Kelp, cut	280172	4
Sanacorp	Kelp, cut	11351105	1
Caelo	Kidney vetch, coarsely rubbed	13104301	2
AHD	Knotgrass	4301A150527	1
Caelo	Knotgrass	4301A100126	2
Caelo	Knotgrass	8111202	1
Caelo	Knotgrass	12295702	3
Caelo	Knotgrass	12295704	4
Caelo	Knotgrass	4312M-01674	1
Caelo	Knotgrass	12368904	1
Caelo	Knotgrass	14079304	1
Caelo	Knotgrass	12368903	1
Caelo	Knotgrass	7102427	1
Caelo	Knotgrass	12368906	3
Finze	Knotgrass	10237202	1
Klenk	Knotgrass	4301A120912	1
Klenk	Knotgrass	4301A121120	4
Caelo	Knotgrass	12368902	5

L

Supplier	Substance	Batch	Spectra
Caelo	Lady's bedstraw herb	10375707	2
Caelo	Lady's bedstraw herb	24101201	1
Caelo	Lady's bedstraw herb	11265102	9
Caelo	Lady's bedstraw herb	7011301	1
Caelo	Lady's bedstraw herb	2401311647	1
Caelo	Lady's bedstraw herb	22041303	1
Caelo	Lady's bedstraw herb	11265104	1
Caelo	Lady's bedstraw herb	14019202	1
Caelo	Lady's bedstraw herb	15029906	1
Caelo	Lady's bedstraw herb	11265103	5
Caelo	Lady's bedstraw herb	10375702	1
Caelo	Lady's bedstraw herb	12369002	3
Caelo	Lady's bedstraw herb	12369006	5
Caelo	Lady's bedstraw herb	12369007	3
Caesar&loretz,Phoenix	Lady's bedstraw herb	14019206	1
Caesar&loretz,Phoenix	Lady's bedstraw herb	14019215	1
Fagron	Lady's bedstraw herb	12369004	2
Galke	Lady's bedstraw herb	21942	2
Caelo	Lady's bedstraw herb	12369001	3
Klenk	Lady's bedstraw herb	3921B12030	1
Klenk	Lady's bedstraw herb	3921C130226	1
Caelo	Lady's bedstraw herb	11265106	3
Sanacorp	Lady's bedstraw herb	11265109	1
Sanacorp	Lady's bedstraw herb	12369003	8
Caelo	Lapacho wood, cut	19061301	1
Caelo	Lapacho wood, cut	13298308	1
Caelo	Lapacho wood, cut	11154506	1
Caelo	Lapacho wood, cut	2x11154506	1
Caelo	Lapacho wood, cut	12239303	2
Caelo	Lapacho wood, cut	12239305	8
Kenk / Phoenix	Lapacho wood, cut	5161A110204	1
Klenk	Lapacho wood, cut	13298302	1
Caelo	Lapacho wood, cut	13298305	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Large waybread herb	14125907	1
Caelo	Large waybread herb	10349610	1
Caelo	Large waybread herb	12374104	7
Caelo	Large waybread herb	123741004	1
Caelo	Large waybread herb	10349614	1
Caelo	Large waybread herb	12374106	2
Caelo	Large waybread herb	13232401	1
Caelo	Large waybread herb	13232404	1
Caelo	Large waybread herb	10349603	2
Caelo	Large waybread herb	10349605	1
Caelo	Large waybread herb	12374101	4
Caelo	Large waybread herb	9311208	1
Klenk	Large waybread herb	4281N110404	1
Klenk	Large waybread herb	N111121	1
Klenk	Large waybread herb	4281N111121	5
Caelo	Laurel leaf	12299106	3
Caelo	Laurel leaf	12299101	1
Klenk	Laurel leaf	B110809	1
Klenk	Laurel leaf, cut	B110809	2
Anzag	Lavender flower	1488A12803	1
Bombastus	Lavender flower	268832	1
Bombastus	Lavender flower	274469	1
Bombastus	Lavender flower	279213	1
Caelo	Lavender flower	11054104	2
Caelo	Lavender flower	15061201	1
Caelo	Lavender flower	15061209	1
Caelo	Lavender flower	11327903	6
Caelo	Lavender flower	11327905	2
Caelo	Lavender flower	27091202	1
Caelo	Lavender flower	12088002	4
Caelo	Lavender flower	12088003	8
Caelo	Lavender flower	12031302	1
Caelo	Lavender flower	12088005	3
Caelo	Lavender flower	19071303	1
Caelo	Lavender flower	6091304	1
Caelo	Lavender flower	13185002	1
Caelo	Lavender flower	13159601	1
Caelo	Lavender flower	13336008	1
Caelo	Lavender flower	13387204	1
Caelo	Lavender flower	11054107	1
Caelo	Lavender flower	11054106	2
Caelo	Lavender flower	12088006	3
Caelo	Lavender flower	1318501	1
Caelo	Lavender flower	13185001-3389311070	1
Caelo	Lavender flower	13185001-3415310152	1
Caelo	Lavender flower	13185006	1
Caelo	Lavender flower	13185001	28
Fagron	Lavender flower	1489A120919	6
Galke	Lavender flower	21416	2
Hepart AG	Lavender flower	A130214	4
Herbasinica	Lavender flower	1488A130830	1
Caelo	Lavender flower	13185003	10
Klenk	Lavender flower	1489A1203	1
Klenk	Lavender flower	1488A111201	2
Klenk	Lavender flower	1488A120803	3
Klenk	Lavender flower	1488B130604	5
Klenk	Lavender flower	313U-01462	1
Klenk	Lavender flower	1489A100125	1
Klenk	Lavender flower	1489A120103	19
Klenk	Lavender flower	1489A130214	16

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Lavender flower	1488B130111	2
Caelo	Lemon grass, cut	13149703	1
Caelo	Lemon grass, cut	13341301	1
Caelo	Lemon grass, cut	11301509	2
Caelo	Lemon grass, cut	11301501	1
Klenk	Lemon grass, cut	7721A130708	1
Klenk	Lemon grass, cut	A120906	1
Klenk	Lemon grass, cut	A130907	1
Klenk	Lemon grass, cut	7721A120906	1
Caelo	Lemon grass, cut	13149701	4
Caelo	Lemon grass, cut	11301503	1
Wolf	Lemon grass, cut	B654	1
Caelo	Lemon peel, cut	12217402	1
Caelo	Lemon peel, cut	12217401	1
Caelo	Lemon peel, cut	12217404	1
Galke	Lemon peel, cut	22975	1
Klenk	Lemon peel, cut	621A130221	1
Klenk	Lemon peel, cut	621A091016	1
Klenk	Lemon peel, cut	B130521	1
Klenk	Lemon peel, cut	A130221	3
Caelo	Lemon verbena leaf, cut	13037702	1
Caelo	Lemon verbena leaf, cut	12137505	1
Caelo	Lemon verbena leaf, cut	12137507	3
Caelo	Lemon verbena leaf, cut	10018208	1
Klenk	Lemon verbena leaf, cut	2411B110408	2
Wolf	Lemon verbena leaf, cut	E-587	1
Wolf	Lemon verbena leaf, cut	B-312	1
Wolf	Lemon verbena leaf, cut	23635	1
Caelo	Lime flower	11086305	7
Bahnhof-Apotheke	Lime flower	7-121011	1
Bombastus	Lime flower	275129	2
Bombastus	Lime flower	280678	3
Caelo	Lime flower	9206604	1
Caelo	Lime flower	10273608	2
Caelo	Lime flower	11086307	3
Caelo	Lime flower	272958	7
Caelo	Lime flower	12170703	1
Caelo	Lime flower	1210702	1
Caelo	Lime flower	10273606	1
Caelo	Lime flower	12170702	2
Caelo	Lime flower	28031302	1
Caelo	Lime flower	Int.Ch:210140	1
Caelo	Lime flower	12170701	1
Caelo	Lime flower	15111301	1
Caelo	Lime flower	13337403	5
Caelo	Lime flower	13101708	1
Caelo	Lime flower	15068302	1
Caelo	Lime flower	268709	2
Caelo	Lime flower	13101701	7
Caelo	Lime flower	12170702-3355319071	1
Caelo	Lime flower	13337403-348012102	1
Caelo	Lime flower	13101702	8
galke,	Lime flower	2098	1
Klenk	Lime flower	1611B120827	11
Klenk	Lime flower	1611B130905	5
Klenk	Lime flower	1611B110421	2
Klenk	Lime flower	Pr.Nr.4411A-01474	1
Klenk	Lime flower	B130307	2
Klenk	Lime flower	1611B1010004	1
Klenk	Lime flower	B130905	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Lime flower	1611B131220	1
Klenk	Lime flower	1611B121105	4
Klenk	Lime flower	1611a121120	2
Klenk	Lime flower	1611A121120	7
Klenk	Lime flower	1611B111011	6
Klenk	Lime flower	1611B130307	4
Phönix	Lime flower	2090413	1
Phönix	Lime flower	1611A12120	1
Sanacorp	Lime flower	264045	1
Wolf	Lime flower	B449	1
Wolf	Lime flower	22094	1
Caelo	Lime leaf, cut	1611A121120	1
Klenk	Lime leaf, cut	2471B120502	1
Akazie	Linseed	20.09.2015	2
Anzag	Linseed	12137105	1
Bombastus	Linseed	1610	1
Bombastus	Linseed	269500	1
Bombastus	Linseed	278457	6
Bombastus	Linseed	274032	1
Bombastus	Linseed	282734	3
Bombastus	Linseed	295376	1
Caelo	Linseed	15061201	1
Caelo	Linseed	12092102	4
Caelo	Linseed	11365508	1
Caelo	Linseed	11365507	1
Caelo	Linseed	12092103	3
Caelo	Linseed	12321601	1
Caelo	Linseed	12092104	2
Caelo	Linseed	28051303	1
Caelo	Linseed	12321602	4
Caelo	Linseed	12321604	2
Caelo	Linseed	11199006	1
Caelo	Linseed	1232006	1
Caelo	Linseed	12382006	3
Caelo	Linseed	12321607	1
Caelo	Linseed	18111302	1
Caelo	Linseed	12321606	2
Caelo	Linseed	13262702	1
Caelo	Linseed	13296702	3
Caelo	Linseed	13262703	3
Caelo	Linseed	28051403	1
Caelo	Linseed	1326703	2
Caelo	Linseed	7370A131104	1
Caelo	Linseed	13140305	1
Caelo	Linseed	13412804	1
Caelo	Linseed	13262704	2
Caelo	Linseed	15053702	1
Caelo	Linseed	13296707	1
Caelo	Linseed	15006005	1
Caelo	Linseed	15006605	1
Caelo	Linseed	15321902	1
Caelo	Linseed	21081703	1
Caelo	Linseed	3923	1
Caelo	Linseed	17067203	1
Caelo	Linseed	12382002	2
Caelo	Linseed	16355404	1
Caelo	Linseed	18007801	2
Caelo	Linseed	18145601	1
Caelo	Linseed	13296705	5
Caelo	Linseed	16040002	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Linseed	17067204	1
Caelo	Linseed	16040005	1
Caelo	Linseed	12186901	2
Caelo	Linseed	16040001	1
Caelo	Linseed	16011403	3
Caelo	Linseed	15006601	2
Caelo	Linseed	15006607	1
Caelo	Linseed	16355401	2
Caelo	Linseed	4713U02240	1
Caelo	Linseed	15006602	2
Caelo	Linseed	7307A170619	2
Caelo	Linseed	3615A-02240	1
Caelo	Linseed	18145603	2
Caelo	Linseed	11199003	1
Caelo	Linseed	7307A141201	3
Fiebig	Linseed	16011405	4
Finze	Linseed	3607E-02240	1
Gehe	Linseed	18145605	1
Hedinger	Linseed	16011402	1
Heinrich Kle/Sanacor	Linseed	7307A170111	3
Klenk	Linseed	1910212240	1
Klenk	Linseed	903312240	1
Klenk	Linseed	7300A111107	4
Klenk	Linseed	7308A111107	3
Klenk	Linseed	7300A130110	7
Klenk	Linseed	1913Q-02240	1
Klenk	Linseed	A130110	1
Klenk	Linseed	7307A130722	5
Klenk	Linseed	7307A-130722	1
Klenk	Linseed	7300A140526	1
Klenk	Linseed	7307A160414	4
Klenk	Linseed	7308A150710	2
Klenk	Linseed	7300A170306	7
Klenk	Linseed	7300A180523	2
Klenk	Linseed	7300A170306-1	1
Klenk	Linseed	7300A141201	6
Klenk	Linseed	7308A150414	2
Klenk	Linseed	7307A150710	6
Klenk	Linseed	7307A170110	2
Klenk	Linseed	7307A130124	1
Klenk	Linseed	7307a131104	1
Klenk	Linseed	7307A140526	3
Klenk	Linseed	7308A130110	4
Klenk	Linseed	2002285	1
Klenk	Linseed	7307A131104	8
Klenk	Linseed	7307A-130110	1
Klenk	Linseed	3707A140526	1
Klenk	Linseed	7500A140556	1
Klenk	Linseed	7300A130722	8
Midas	Linseed	7308A161208	1
Noweda	Linseed	7307A111107	7
Klenk	Linseed	7307a111107	1
Klenk	Linseed	7307A121212	1
Caelo	Linseed	12382004	1
Klenk	Linseed	7307A131021	1
Phonix	Linseed	13296703	3
Klenk	Linseed	7307A150414	1
Caelo	Linseed	16355402	7
Klenk	Linseed	7307A130110	15
aurica/phoenix	Liqourice root	521206925	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Liqourice root	2901312151	1
Bombastus	Liqourice root	903312151	1
Bombastus	Liqourice root	279409	2
Bombastus	Liqourice root	5091305	1
Bombastus	Liqourice root	285185	2
Bombastus	Liqourice root	286584	1
Bombastus	Liqourice root	278377	3
Bombastus	Liqourice root	274921	3
Bombastus	Liqourice root	3713Q2151	1
Caelo	Liqourice root	13037904	1
Caelo	Liqourice root	10110912	1
Caelo	Liqourice root	12267103	1
Caelo	Liqourice root	13037902	1
Caelo	Liqourice root		1
Caelo	Liqourice root	12267104	2
Gehe	Liqourice root	277004	2
Gehe	Liqourice root	283316	1
Gehe	Liqourice root	284243	2
Klenk	Liqourice root	6391A080905	4
Klenk	Liqourice root	6391A110421	4
Klenk	Liqourice root	6390A101020	1
PHOENIX am 27.12.2013	Liqourice root	281844	1
Bombastus	Liqourice root	276468	6
Phönix	Liqourice root	276425	1
Bahnhof-Apotheke	Liqourice root, peeled	17-121112	1
Bombastus	Liqourice root, peeled	268001	1
Bombastus	Liqourice root, peeled	270192	1
Caelo	Liqourice root, peeled	6381A111004	14
Caelo	Liqourice root, peeled	1135904	1
Caelo	Liqourice root, peeled	11351911	4
Caelo	Liqourice root, peeled	10011301	1
Caelo	Liqourice root, peeled	1351911	1
Caelo	Liqourice root, peeled	11351913	1
Caelo	Liqourice root, peeled	11351910	2
Caelo	Liqourice root, peeled	638a120806	1
Caelo	Liqourice root, peeled	13104503	3
Caelo	Liqourice root, peeled	13104504	4
Caelo	Liqourice root, peeled	18121302	1
Caelo	Liqourice root, peeled	13194101	5
Caesar & Loretz Gm...	Liqourice root, peeled	11034014	1
Galke	Liqourice root, peeled	23538	1
Gehe	Liqourice root, peeled	268835	1
Gehe	Liqourice root, peeled	270853	3
Gehe	Liqourice root, peeled	1250213	1
Caelo	Liqourice root, peeled	12227112	1
Klenk	Liqourice root, peeled	6381a111004	1
Klenk	Liqourice root, peeled	6381A121126	27
Klenk	Liqourice root, peeled	6381A130426	21
Klenk	Liqourice root, peeled	A130426	1
Klenk	Liqourice root, peeled	A130820	3
Klenk	Liqourice root, peeled	6381A130820	4
Klenk	Liqourice root, peeled	6381A140109	2
Klenk	Liqourice root, peeled	6381A130425	1
Klenk	Liqourice root, peeled	6381A110531	2
Klenk	Liqourice root, peeled	638A130820	1
Klenk	Liqourice root, peeled	6381a121126	1
Noweda	Liqourice root, peeled	70226/1	1
Klenk	Liqourice root, peeled	6381A120806	3
Phoenix	Liqourice root, peeled	6381A120611	12

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Liqourice root, peeled	11351906	3
Caelo	Liqourice root, peeled	277004	1
Caelo	Liqourice root, peeled	11351905	3
Bombastus	Lovage root	273001	1
Caelo	Lovage root	11181609	3
Caelo	Lovage root	12189001	1
Caelo	Lovage root	11181611	3
Caelo	Lovage root	4312M-02150	1
Caelo	Lovage root	12169007	1
Caelo	Lovage root	12169009	1
Caelo	Lovage root	12169012	1
Caelo	Lovage root	13385005	1
Caelo	Lovage root	12189002	1
Caelo	Lovage root	107063	1
Caelo	Lovage root	12169008	4
Caelo	Lovage root	12169006	3
Caelo	Lovage root	12169002	2
Caelo	Lovage root	12169010	2
Klenk	Lovage root	6371A080508	1
Klenk	Lovage root	B110228	1
Klenk	Lovage root	B121029	1
Klenk	Lovage root	6371B-121029	1
Klenk	Lovage root	6371B121029	3
Caelo	Lungwort herb, cut	11021707	1
Caelo	Lungwort herb, cut	11134203	12
Caelo	Lungwort herb, cut	4331b111205	1
Caelo	Lungwort herb, cut	13029302	25
Caelo	Lungwort herb, cut	11134205	3
Caelo	Lungwort herb, cut	11134201	1
Caelo	Lungwort herb, cut	13029306	3
Caelo	Lungwort herb, cut	11021709	2
Caelo	Lungwort herb, cut	13355801	2
Caesar & Loretz Gm...	Lungwort herb, cut	13029304	5
Fagron	Lungwort herb, cut	Nachprüfung	1
Galke	Lungwort herb, cut	19511	4
Klenk	Lungwort herb, cut	4331B111205	1
Klenk	Lungwort herb, cut	4331A120813	1
Richter	Lungwort herb, cut	P195884	1
Caelo	Lungwort herb, cut	11134202	3
Caelo	Lycopodium herb	11255012	2
Bahnhof-Apotheke	Lycopodium herb	17-121112	1
Caelo	Lycopodium herb	11255003	1
Caelo	Lycopodium herb	9378812	1
Caelo	Lycopodium herb	11255005	3
Caelo	Lycopodium herb	11255008	12
Caelo	Lycopodium herb	11255009	3
Caelo	Lycopodium herb	11255011	5
Caelo	Lycopodium herb	11255014	7
Caelo	Lycopodium herb	11255010	1
Caelo	Lycopodium herb	11255016	2
Caelo	Lycopodium herb	11255018	1
Caelo	Lycopodium herb	13101501	1
Caelo	Lycopodium herb	1310502	1
Caesar/Noweda	Lycopodium herb	1255008	1
Finze	Lycopodium herb	9378803	1
Galke	Lycopodium herb	16913	3
Klenk	Lycopodium herb	4111B120220	1
Klenk	Lycopodium herb	4111B110428	1
Caelo	Lycopodium herb	11255017	6
Sanacorp	Lycopodium herb	13101502	2

M

Supplier	Substance	Batch	Spectra
Fagron	Macrogols 6000 powder	14J17-B01	1
Fagron	Macrogols 6000 powder	12J22-N02	1
Fagron	Macrogols 6000 powder	11G14-N03	1
Fagron	Magnesium aspartate dihydrate	17C21-B05-333111	1
Caelo	Magnesium carbonate, heavy	2091303	1
Caelo	Magnesium carbonate, heavy	13123505	1
Caelo	Magnesium carbonate, heavy	13123502	1
Caelo	Magnesium carbonate, heavy	7011404	1
Caelo	Magnesium carbonate, heavy	13123504	2
Caelo	Magnesium carbonate, heavy	12135404	1
Euro OTC	Magnesium carbonate, heavy	1305024-01	1
Fagron	Magnesium carbonate, heavy	12F20-N04	1
Euro OTC	Magnesium carbonate, heavy	1211005-01	4
Euro OTC	Magnesium oxide, heavy	1205012-01	1
Euro OTC	Magnesium oxide, heavy	1012033-01	1
Caelo	Magnesium sulfate, dried	11265902	1
Caelo	Magnesium sulfate, dried	11265903	1
Caelo	Magnesium sulfate, dried	12157202	1
Caelo	Magnesium sulfate, dried	M-220413-2	1
Caelo	Magnesium sulfate, dried	12157207	1
Caelo	Magnesium sulfate, dried	12157208	1
Caelo	Magnesium sulfate, dried	10213213	2
Caelo	Magnesium sulfate, dried	11265908	2
Anzag	Maize style	274920	1
Aurica/Phönix	Maize style	520901387	1
Bahnhof-Apotheke	Maize style	20-121018	1
Bombastus	Maize style	282574	1
Bombastus	Maize style	285912	1
Bombastus	Maize style	276776	1
Bombastus	Maize style	81113a	1
Bombastus	Maize style	17001482	1
Bombastus	Maize style	19002817	1
Caelo	Maize style	10325902	2
Caelo	Maize style	10325906	7
Caelo	Maize style	10325904	1
Caelo	Maize style	10325907	4
Caelo	Maize style	10325905	1
Caelo	Maize style	280363	1
Caelo	Maize style	11280404	2
Caelo	Maize style	13277201	1
Caelo	Maize style	13277202	1
Caelo	Maize style	13277207	1
Caelo	Maize style	11280405	11
Caelo	Maize style	13277205	1
Caelo	Maize style	15226102	1
Caelo	Maize style	15226103	1
Gehe	Maize style	18041004	1
Klenk	Maize style	5581A081204	1
Klenk	Maize style	5581A111206	1
Klenk	Maize style	A110411	1
Richter	Maize style	B189316	1
Sana 21.10.14 Ek 3.57	Maize style	13381603	2
A.H. 27.05.13 ek: 6,75EUR	Male speedwell wort	274239	1
Anzag ek: 4,88EUR 26…	Male speedwell wort	4661C120321	10
Aurica/Phönix	Male speedwell wort	520708362	1
Bahnhof-Apotheke	Male speedwell wort	4-121002	1
Bombastus	Male speedwell wort	274238	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Male speedwell wort	12162503	1
Caelo	Male speedwell wort	11265503	5
Caelo	Male speedwell wort	11265502	1
Caelo	Male speedwell wort	4661c111011	1
Caelo	Male speedwell wort	3051306	1
Caelo	Male speedwell wort	12162504	13
Caelo	Male speedwell wort	11061305	1
Caelo	Male speedwell wort	28061303	1
Caelo	Male speedwell wort	3091305	1
Caelo	Male speedwell wort	13166701	3
Caelo	Male speedwell wort	14111303	1
Caelo	Male speedwell wort	20111303	1
Caelo	Male speedwell wort	1216504	1
Caelo	Male speedwell wort	12162505	2
Finze	Male speedwell wort	4661B080915	1
Klenk	Male speedwell wort	4661A090318	1
Klenk	Male speedwell wort	4661B110916	1
Klenk	Male speedwell wort	4661C120802	13
Klenk	Male speedwell wort	4661C130226	27
Klenk	Male speedwell wort	C120321	1
Klenk	Male speedwell wort	C130226	5
Klenk	Male speedwell wort	4661C13026	1
Klenk	Male speedwell wort	4661C131104	1
Klenk	Male speedwell wort	4661C111011	13
Klenk	Male speedwell wort	4661B101011	1
Klenk	Male speedwell wort	4661C130226-32743106	1
Klenk	Male speedwell wort	4661c130226-34343111	1
Klenk	Male speedwell wort	4661C2004	1
Klenk	Male speedwell wort	4661C-111011	1
Klenk	Male speedwell wort	4661B110121	2
Klenk	Male speedwell wort	6661C130226	1
Klenk	Male speedwell wort	4661c120802	1
Klenk	Male speedwell wort	4661c120321	1
Phönix	Male speedwell wort	13089201	4
Bombastus	Mallow flower	273803	1
Bombastus	Mallow flower	13267304	1
Caelo	Mallow flower	20061201	1
Caelo	Mallow flower	10357902	1
Caelo	Mallow flower	11040106	4
Caelo	Mallow flower	8121202	1
Caelo	Mallow flower	27021301	1
Caelo	Mallow flower	12187405	4
Caelo	Mallow flower	12187404	4
Caelo	Mallow flower	12187501	6
Caelo	Mallow flower	12187502	1
Caelo	Mallow flower	13040402	1
Caelo	Mallow flower	18111303	1
Caelo	Mallow flower	13267303	2
Caelo	Mallow flower	13267302	1
Caelo	Mallow flower	13351309	1
Caelo	Mallow flower	13351307	1
Caelo	Mallow flower	10357904	1
Caelo	Mallow flower	13351301	2
Caelo	Mallow flower	13351303	2
Caelo	Mallow flower	9311104	1
Caelo	Mallow flower	13267301-3409310112	1
Caelo	Mallow flower	12187501-3414310132	1
Caesar & Loretz Gm…	Mallow flower	12187402	8
Caesar & Loretz Gm…	Mallow flower	13267301	6
Galke	Mallow flower	21119	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Gehe	Mallow flower	1501B110207	1
Gehe	Mallow flower	1501B120508	6
Klenk	Mallow flower	10357908	2
Caelo	Mallow flower	12187505	3
Klenk	Mallow flower	1910211464	1
Klenk	Mallow flower	1501B120427	10
Klenk	Mallow flower	1501B111215	1
Klenk	Mallow flower	1501B-120427	1
Klenk	Mallow flower	B120427	1
Klenk	Mallow flower	B130829	3
Klenk	Mallow flower	1501b111215	1
Klenk	Mallow flower	1501B130829	3
Klenk	Mallow flower	150B111215	1
Klenk	Mallow flower	1501B100408	1
Nachprüfung 29.10.12	Mallow flower	C1316	1
Klenk	Mallow flower	1501b110207	1
Caelo	Mallow leaf	28061203	1
Caelo	Mallow leaf	2131B120529	3
Caelo	Mallow leaf	12310001	3
Caelo	Mallow leaf	12310004	4
Caelo	Mallow leaf	12310009	2
Caelo	Mallow leaf	12310008	1
Caelo	Mallow leaf	20111302	1
Caelo	Mallow leaf	14073902	1
Caelo	Mallow leaf	13174213	1
Caelo	Mallow leaf	12153403	1
Caelo	Mallow leaf	10290515	1
Caelo	Mallow leaf	10290502	1
Caelo	Mallow leaf	13174207	1
Galke	Mallow leaf	17133	1
Galke	Mallow leaf	21454	1
Galke	Mallow leaf	21445	1
Gehe	Mallow leaf	2131B110420	2
Gehe	Mallow leaf	10290512	1
Klenk	Mallow leaf	2131B10529	1
Klenk	Mallow leaf	2131B130225	4
Klenk	Mallow leaf	B130225	1
Sanacorp	Mallow leaf	278925	1
Caelo	Mallow leaf	13174217	1
Caelo	Mallow leaf	12310006	1
Anzag ek:8.77EUR 30.08.12	Manna	11308904	2
Caelo	Manna	11308901	2
Caelo	Manna	11308909	2
Caelo	Manna	25111301	1
Caelo	Manna	11041401	1
Caelo	Manna	11061404	1
Caelo	Manna	25071403	1
Caelo	Manna	28101404	1
Caelo	Manna	13041712	1
Caelo	Manna	15219010	3
Caelo	Manna	15111738	1
Caelo	Manna	11308907	2
Caelo	Manna	13127003	5
Caelo	Manna	11308911	2
Caelo	Manna	15219005	1
Caelo	Manna	14001303	3
Caelo	Manna	14001310	3
Caelo	Manna	15219003	3
Caelo	Manna	15219008	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Manna	5221A110817	1
Klenk	Manna	5221A140210	4
Klenk	Manna	5221A150107	2
Caelo	Manna	15219012	1
Klenk	Manna	5221A120509	10
Caelo	Manna	15219009	1
Caelo	Manna, powdered	11308802	2
Caelo	Manna, powdered	11003611	1
Caelo	Manna, powdered	11071311	1
Caelo	Manna, powdered	15101306	1
Caelo	Manna, powdered	15101312	1
Caelo	Manna, powdered	11308807	1
Caelo	Manna, powdered	14001402	1
Caelo	Manna, powdered	14001408	1
Galke	Manna, powdered	20669	1
Galke	Manna, powdered	19784	1
Noweda	Manna, powdered	11170102	1
Bombastus	Marian thistle fruit	296535	1
Bombastus	Marian thistle fruit	296193	1
Bombastus	Marian thistle fruit	299483	1
Bombastus	Marian thistle fruit	269499	1
Bombastus	Marian thistle fruit	280304	1
Bombastus	Marian thistle fruit	278379	1
Bombastus	Marian thistle fruit	282283	1
Bombastus	Marian thistle fruit	282034	2
Bombastus	Marian thistle fruit	279405	3
Bombastus	Marian thistle fruit	277720	3
Bombastus	Marian thistle fruit	278378	1
Bombastus	Marian thistle fruit	284420	1
Bombastus	Marian thistle fruit	13122013a	1
Caelo	Marian thistle fruit	12189116	2
Caelo	Marian thistle fruit	10270613	1
Caelo	Marian thistle fruit	11126702	9
Caelo	Marian thistle fruit	10270614	2
Caelo	Marian thistle fruit	27111203	1
Caelo	Marian thistle fruit	1126703	1
Caelo	Marian thistle fruit	11126701	1
Caelo	Marian thistle fruit	1126705	1
Caelo	Marian thistle fruit	11126705	1
Caelo	Marian thistle fruit	12189106	4
Caelo	Marian thistle fruit	12189104	2
Caelo	Marian thistle fruit	12189105	1
Caelo	Marian thistle fruit	12189109	2
Caelo	Marian thistle fruit	12189113	6
Caelo	Marian thistle fruit	12189111	3
Caelo	Marian thistle fruit	12189115	2
Caelo	Marian thistle fruit	18111301	1
Caelo	Marian thistle fruit	13326202	3
Caelo	Marian thistle fruit	15409204	2
Caelo	Marian thistle fruit	12198107	1
Caelo	Marian thistle fruit	12189107	2
Caelo	Marian thistle fruit	12189108	4
Caelo	Marian thistle fruit	11126703	2
Caelo	Marian thistle fruit	1289112	1
ebert u.jacobi	Marian thistle fruit	287527	1
Galke	Marian thistle fruit	22187	4
Klenk	Marian thistle fruit	7180A090929	1
Klenk	Marian thistle fruit	7180A120725	1
Klenk	Marian thistle fruit	A120725	1
Klenk	Marian thistle fruit	7180A130219	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Marian thistle fruit	7180A132019	1
Klenk	Marian thistle fruit	7180A110209	2
Caelo	Marian thistle fruit	12189112	5
Caelo	Marian thistle herb	10365604	4
Caelo	Marian thistle herb	10315909	1
Caelo	Marian thistle herb	10315911	4
Caelo	Marian thistle herb	10315907	1
Caelo	Marian thistle herb	17121204	1
Caelo	Marian thistle herb	10365601	4
Caelo	Marian thistle herb	1035911	1
Caelo	Marian thistle herb	18041303	1
Caelo	Marian thistle herb	intch:318080	1
Caelo	Marian thistle herb	13130703	2
Caelo	Marian thistle herb	1313702	1
Caelo	Marian thistle herb	30101306	1
Caelo	Marian thistle herb	13130701	2
Caelo	Marian thistle herb	13130704	5
Caelo	Marian thistle herb	10365605	1
Caelo	Marian thistle herb	62607127	1
Caelo	Marian thistle herb	13130701-3492411030	1
Caelo	Marian thistle herb	13386703-3543411013	1
Caelo	Marian thistle herb	13130702	3
Euro OTC	Marian thistle herb	3701A-111207	1
Gehe	Marian thistle herb	10365602	2
Klenk	Marian thistle herb	3701B130318	5
Klenk	Marian thistle herb	11041310	1
Klenk	Marian thistle herb	3701B111117	1
Klenk	Marian thistle herb	B110728	1
Klenk	Marian thistle herb	3701a111207	1
Klenk	Marian thistle herb	2011402	1
Klenk	Marian thistle herb	3701A100916	2
Klenk	Marian thistle herb	913E-01627	1
Klenk	Marian thistle herb	3701A111207	11
Klenk	Marian thistle herb	3701B120717	3
Caelo	Marjoram herb	12168901	3
Caelo	Marjoram herb	11212711	3
Caelo	Marjoram herb	12168903	10
Caelo	Marjoram herb	12168905	2
Caelo	Marjoram herb	12168904	1
Caelo	Marjoram herb	12168908	6
Caelo	Marjoram herb	6051302	1
Caelo	Marjoram herb	12168907	3
Caelo	Marjoram herb	12168912	1
Caelo	Marjoram herb	27011402	1
Caelo	Marjoram herb	11212707	1
Caelo	Marjoram herb	12168906	1
Caelo	Marjoram herb	13113304	3
Caelo	Marjoram herb	12168909	6
Caelo	Marjoram herb	13113303	3
Caelo	Marjoram herb	12168902	1
Caelo	Marjoram herb	12168910	8
Caelo	Marjoram herb	9292602	1
Caesar&loretz,Phoenix	Marjoram herb	14181005	1
Galke	Marjoram herb	22401	1
Galke	Marjoram herb	23241	1
Klenk	Marjoram herb	4881A101025	15
Klenk	Marjoram herb	A101025	2
Klenk	Marjoram herb	4881A1311105	1
Klenk	Marjoram herb	4881a101025	1
Klenk	Marjoram herb	12345678	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Marjoram herb	4881A100929	3
Wolf	Marjoram herb	163516	1
Wolf	Marjoram herb	B163516	6
Wolf	Marjoram herb	P232243	9
Caelo	Marrubium vulgare herb, cut	1153803	1
Caelo	Marrubium vulgare herb, cut	12231604	4
Caelo	Marrubium vulgare herb, cut	313091	1
Caelo	Marrubium vulgare herb, cut	13289109	1
Caelo	Marrubium vulgare herb, cut	11253802	1
Caelo	Marrubium vulgare herb, cut	12231603	1
Caelo	Marrubium vulgare herb, cut	12231601	4
Caelo	Marrubium vulgare herb, cut	11253803	1
Caelo	Marrubium vulgare herb, cut	12231605	4
Klenk	Marrubium vulgare herb, cut	4141A130110	1
Klenk	Marrubium vulgare herb, cut	13289102	1
Noweda	Marrubium vulgare herb, cut	4141A080513	1
Caelo	Marshmallow leaf	12328202	3
Caelo	Marshmallow leaf	12328206	3
Caelo	Marshmallow leaf	13199604	4
Caelo	Marshmallow leaf	12328207	2
Bombastus	Marshmallow root	273458	1
Caelo	Marshmallow root	26091201	1
Caelo	Marshmallow root	11101907	7
Caelo	Marshmallow root	11101804	1
Caelo	Marshmallow root	6071A130116	10
Caelo	Marshmallow root	12147311	1
Caelo	Marshmallow root	12147311	7
Caelo	Marshmallow root	13057103	1
Caelo	Marshmallow root	12368906	1
Caelo	Marshmallow root	15104503	1
Caelo	Marshmallow root	11101905	1
Caelo	Marshmallow root	11101804	1
Gehe	Marshmallow root	6071A120306	2
Klenk	Marshmallow root	6071A130612	4
Klenk	Marshmallow root	6074B100416	1
Klenk	Marshmallow root	6071A120314	10
Klenk	Marshmallow root	6071A-130408	1
Klenk	Marshmallow root	A130408	3
Klenk	Marshmallow root	6071A-120314	1
Klenk	Marshmallow root	130116	1
Klenk	Marshmallow root	6071a130408	1
Klenk	Marshmallow root	6071B091207	1
Phönix	Marshmallow root	6071a120314	1
Phönix	Marshmallow root	2090413	1
Phönix	Marshmallow root	6071A130408	14
Bombastus	Marshmallow root, natural	270467	1
Bombastus	Marshmallow root, natural	276741	1
Caelo	Marshmallow root, natural	270114	1
Caelo	Masterwort root, cut	1210801	1
Caelo	Masterwort root, cut	12101806	2
Caelo	Masterwort root, cut	12101808	1
Caelo	Masterwort root, cut	13132002	1
Caelo	Masterwort root, cut	13341201	1
Caelo	Masterwort root, cut	12101807	2
Galke	Masterwort root, cut	18411	1
Galke	Masterwort root, cut	23074	1
Caelo	Maté leaf	12133803	3
Caelo	Maté leaf	2141A120821	2
Caelo	Maté leaf	13061202	1
Caelo	Maté leaf	12133806	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Maté leaf	13118003	4
Caelo	Maté leaf	12133801	3
Caelo	Maté leaf	11091710	1
Caelo	Maté leaf	12133804	7
Caelo	Maté leaf	13118001	1
Caelo	Maté leaf	12133807	7
Caesar & Loretz Gm…	Maté leaf	13118002	10
Galke	Maté leaf	22365	1
Klenk	Maté leaf	2141A111213	16
Klenk	Maté leaf	2131A111213	1
Klenk	Maté leaf	2141A-111213	1
Klenk	Maté leaf	2141a111213	1
Klenk	Matricaria flower	1290A-120620	1
Bahnhof-Apotheke	Matricaria flower	11-121024	1
Bombastus	Matricaria flower	268712	1
Bombastus	Matricaria flower	274106	1
Bombastus	Matricaria flower	273667	1
Bombastus	Matricaria flower	276095	5
Bombastus	Matricaria flower	276307	1
Bombastus	Matricaria flower	271781	1
Bombastus	Matricaria flower	281103	2
Bombastus	Matricaria flower	287855	1
Bombastus	Matricaria flower	299185	1
Bombastus	Matricaria flower	283710	2
Bombastus	Matricaria flower	274105	1
Bombastus	Matricaria flower	273388	1
Bombastus	Matricaria flower	277997	1
Bombastus	Matricaria flower	265419	1
Bombastus	Matricaria flower	268408	1
Bombastus	Matricaria flower	268408	1
Bombastus	Matricaria flower	292757	1
Bombastus	Matricaria flower	277959	2
Bombastus	Matricaria flower	264997	1
Caelo	Matricaria flower	12294802	15
Caelo	Matricaria flower	12294804	1
Caelo	Matricaria flower	11169607	1
Caelo	Matricaria flower	13061201	1
Caelo	Matricaria flower	10081201	1
Caelo	Matricaria flower	22081202	1
Caelo	Matricaria flower	12059606	2
Caelo	Matricaria flower	5081201	1
Caelo	Matricaria flower	12244802	4
Caelo	Matricaria flower	27091203	1
Caelo	Matricaria flower	11214810	1
Caelo	Matricaria flower	11101203	1
Caelo	Matricaria flower	17101204	1
Caelo	Matricaria flower	12244803	3
Caelo	Matricaria flower	12111903	2
Caelo	Matricaria flower	13111201	1
Caelo	Matricaria flower	16111202	1
Caelo	Matricaria flower	19111207	1
Caelo	Matricaria flower	22111201	1
Caelo	Matricaria flower	22111202	1
Caelo	Matricaria flower	12299701	1
Caelo	Matricaria flower	22011303	1
Caelo	Matricaria flower	12299703	2
Caelo	Matricaria flower	20021313	1
Caelo	Matricaria flower	13031306	1
Caelo	Matricaria flower	19041306	1
Caelo	Matricaria flower	12361701	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Matricaria flower	12337605	2
Caelo	Matricaria flower	13014501	1
Caelo	Matricaria flower	12337601	1
Caelo	Matricaria flower	IntCh:313011	1
Caelo	Matricaria flower	26081303	1
Caelo	Matricaria flower	12337610	1
Caelo	Matricaria flower	12361704	1
Caelo	Matricaria flower	12337608	1
Caelo	Matricaria flower	12361707	2
Caelo	Matricaria flower	13210901	3
Caelo	Matricaria flower	12361706	1
Caelo	Matricaria flower	13011406	1
Caelo	Matricaria flower	13288405	3
Caelo	Matricaria flower	14276804	3
Caelo	Matricaria flower	15090003	2
Caelo	Matricaria flower	15258504	1
Caelo	Matricaria flower	15258505	1
Caelo	Matricaria flower	11218501	1
Caelo	Matricaria flower	13210906	1
Caelo	Matricaria flower	12361702	6
Caelo	Matricaria flower	12361707	4
Caelo	Matricaria flower	13210905	3
Caelo	Matricaria flower	17338903	1
Caelo	Matricaria flower	18290002	1
Caelo	Matricaria flower	12244803	1
Caelo	Matricaria flower	13210901-3478312171	1
Caelo	Matricaria flower	12337607	2
Caelo	Matricaria flower	12244805	4
Caelo	Matricaria flower	12244804	2
Caelo	Matricaria flower	12361706	3
Caelo	Matricaria flower	13210905	1
Caelo	Matricaria flower	18193705	1
Caelo	Matricaria flower	13210903	1
Caelo	Matricaria flower	13210901-3546411013	1
Caelo	Matricaria flower	AKD5	1
Defektur	Matricaria flower	56/12	1
Defektur	Matricaria flower	10/13	1
Defektur	Matricaria flower	29/13	1
Defektur	Matricaria flower	59/13	1
Fagron	Matricaria flower		1
Finze	Matricaria flower	1290B101122	1
Finze	Matricaria flower	12361703	6
Galke	Matricaria flower	18471	5
Galke	Matricaria flower	18803	1
Galke	Matricaria flower	21652	1
Gehe	Matricaria flower	11214802	1
Gehe	Matricaria flower	11255204	1
Gehe	Matricaria flower	12133009	1
Hepart AG	Matricaria flower	B-477,kbA	1
Klenk	Matricaria flower	1290B140123	2
k	Matricaria flower	1290A140513	1
Klenk	Matricaria flower	1290A150618	1
Klenk	Matricaria flower	1290A20404	1
Klenk	Matricaria flower	1290A120404	1
Klenk	Matricaria flower	1290A120404	6
Klenk	Matricaria flower	2310211452	1
Klenk	Matricaria flower	27111204	1
Klenk	Matricaria flower	1290A120403	3
Klenk	Matricaria flower	1290A12061	1
Klenk	Matricaria flower	1290A110825	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Matricaria flower	1290B130415	39
Klenk	Matricaria flower	1290A120601	2
Klenk	Matricaria flower	B130415	2
Klenk	Matricaria flower	11101302	1
Klenk	Matricaria flower	14111314	1
Klenk	Matricaria flower	A130502	1
Klenk	Matricaria flower	A130516	1
Klenk	Matricaria flower	A120529	1
Klenk	Matricaria flower	16121301	1
Klenk	Matricaria flower	1290A130516	3
Klenk	Matricaria flower	1290A130502	1
Klenk	Matricaria flower	1290A130516	9
Klenk	Matricaria flower	A120529	1
Klenk	Matricaria flower	1290A130502	1
Klenk	Matricaria flower	1290B140624	1
Klenk	Matricaria flower	1290A140508	1
Klenk	Matricaria flower	1290A120620	13
Klenk	Matricaria flower	1290A120529	1
Klenk	Matricaria flower	4100113002	2
Klenk	Matricaria flower	1290A120601	14
Klenk	Matricaria flower	1290A180709	1
Klenk	Matricaria flower	1290A110421	1
Klenk	Matricaria flower	1290B130415	3
Klenk	Matricaria flower	1290a120620	1
Klenk	Matricaria flower	1290A110607	1
Klenk	Matricaria flower	1290A120529	5
Phönix	Matricaria flower	1300A120426	1
Sanacorp	Matricaria flower	12294804	6
Sanacorp	Matricaria flower	12294809	3
Sanacorp	Matricaria flower	1300A120725	2
Sanacorp	Matricaria flower	1290B140123	2
Spangropharm	Matricaria flower	11169606	1
Wolf	Matricaria flower	23242	1
-	Meadowsweet	1511M-01685	1
-	Meadowsweet	130849	1
Anzag	Meadowsweet	10381604	5
Caelo	Meadowsweet	10381602	3
Caelo	Meadowsweet	10381601	1
Caelo	Meadowsweet	12188704	2
Caelo	Meadowsweet	12188703	1
Caelo	Meadowsweet	12188803	10
Caelo	Meadowsweet	4912E-01685	1
Caelo	Meadowsweet	12188801	1
Caelo	Meadowsweet	12188807	1
Caelo	Meadowsweet	12188702	1
Caelo	Meadowsweet	12188805	13
Caelo	Meadowsweet	12188806	3
Caelo	Meadowsweet	62487517	1
Galke	Meadowsweet	20358	1
Sanacorp	Meadowsweet	4541A120313	2
Weltecke	Meadowsweet	67010413	1
Caelo	Meadowsweet flower, rubbed	9326211	2
Caelo	Meadowsweet flower, rubbed	9326213	2
Caelo	Meadowsweet flower, rubbed	10349305	1
Caelo	Meadowsweet flower, rubbed	1227501	1
Caelo	Meadowsweet flower, rubbed	12275701	2
Caelo	Meadowsweet flower, rubbed	10051301	1
Caelo	Meadowsweet flower, rubbed	10349308	1
Caelo	Meadowsweet flower, rubbed	1225702	1
Caelo	Meadowsweet flower, rubbed	12275703	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Meadowsweet flower, rubbed	12275704	4
Caelo	Meadowsweet flower, rubbed	12275702	1
Caelo	Meadowsweet flower, rubbed	10349302	2
Caelo	Meadowsweet flower, rubbed	10349307	2
Caelo	Meadowsweet flower, rubbed	12275704-3372319032	1
Klenk	Meadowsweet flower, rubbed	A120312	1
Kräuter Schulte	Meadowsweet flower, rubbed	51369	1
Kräuter Schulte	Meadowsweet flower, rubbed	53473	1
-	Melilot	811Q-01664	1
Anzag ek:3,13EUR 15.09.12	Melilot	11307605	4
Caelo	Melilot	8061204	1
Caelo	Melilot	19071201	1
Caelo	Melilot	24081202	1
Caelo	Melilot	11307606	6
Caelo	Melilot	11307601	1
Caelo	Melilot	12231703	3
Caelo	Melilot	12289202	8
Caelo	Melilot	11307607	1
Caelo	Melilot	122891202	1
Caelo	Melilot	12289203	5
Caelo	Melilot	25091301	1
Caelo	Melilot	22111303	1
Caelo	Melilot	12289206	1
Caelo	Melilot	12289207	1
Caelo	Melilot	12289201	1
Caelo	Melilot	12231701	3
Caelo	Melilot	107063	1
Caelo	Melilot	12289205	4
Gehe	Melilot	110324	1
Klenk	Melilot	4151A110324	8
Klenk	Melilot	4151A120912	1
Klenk	Melilot	A110324	6
Phönix	Melilot	1237903	1
-	Mellisa leaf	131146	1
Alfred Galke	Mellisa leaf	D-NI-1-9516-BC	1
Bahnhof-Apotheke	Mellisa leaf	17-120917	1
Bombastus	Mellisa leaf	270044	1
Bombastus	Mellisa leaf	271499	2
Bombastus	Mellisa leaf	277722	1
Caelo	Mellisa leaf		1
Caelo	Mellisa leaf	1009	1
Caelo	Mellisa leaf	CH.111111	1
Caelo	Mellisa leaf	12032303	1
Caelo	Mellisa leaf	12032309	1
Caelo	Mellisa leaf	12032307	2
Caelo	Mellisa leaf	12032316	3
Caelo	Mellisa leaf	12032312	1
Caelo	Mellisa leaf	25021301	1
Caelo	Mellisa leaf	12032319	5
Caelo	Mellisa leaf	19041303	1
Caelo	Mellisa leaf	25061303	1
Caelo	Mellisa leaf	13030805	1
Caelo	Mellisa leaf	14111319	1
Caelo	Mellisa leaf	24011407	1
Caelo	Mellisa leaf	13214705	1
Caelo	Mellisa leaf	13214720	1
Caelo	Mellisa leaf	10310919	1
Caelo	Mellisa leaf	12032318	1
Caelo	Mellisa leaf	13030803	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Mellisa leaf	2161a121009	1
galke	Mellisa leaf	20867	1
Gehe	Mellisa leaf	12032314	4
Klenk	Mellisa leaf	2161A121206	2
Klenk	Mellisa leaf	2161A151209	1
Klenk	Mellisa leaf	111207	1
Klenk	Mellisa leaf	2807211503	1
Klenk	Mellisa leaf	2161A111207	15
Klenk	Mellisa leaf	2161A110818	1
Klenk	Mellisa leaf	27091201	1
Klenk	Mellisa leaf	2161A120718	11
Klenk	Mellisa leaf	2161A121009	14
Klenk	Mellisa leaf	2161A121009/PN:1198	1
Klenk	Mellisa leaf	2161A121029	4
Klenk	Mellisa leaf	2161A101216	1
Caelo	Mellisa leaf	13214707	1
Caelo	Mellisa leaf	12032310	1
	Methadone hydrochloride	22E02-F04	1
	Methadone hydrochloride	21003277020	2
	Methadone hydrochloride	21003277024	9
	Methadone hydrochloride	22E02-F04-382620	2
	Methadone hydrochloride	23A25-F02-384702	2
	Methadone hydrochloride	23A25-F02-384698	2
	Methadone hydrochloride	23001353006	1
	Methadone hydrochloride	23A25-F02-384693	1
	Methadone hydrochloride	23001356001	1
	Methadone hydrochloride	23003258005	1
Fagron	Methadone hydrochloride	18G02-B02-355989	9
Bombastus	Methadone hydrochloride	14C24-B01-292858	6
ca	Methadone hydrochloride	18132403	11
Caelo	Methadone hydrochloride	15244702	1
Caelo	Methadone hydrochloride	16135312	3
Caelo	Methadone hydrochloride	16135311	4
Caelo	Methadone hydrochloride	1081801	1
Caelo	Methadone hydrochloride	10076407	1
Caelo	Methadone hydrochloride	11227507	1
Caelo	Methadone hydrochloride	12171907	1
Caelo	Methadone hydrochloride	12171902	1
Caelo	Methadone hydrochloride	12171914	1
Caelo	Methadone hydrochloride	17011406	1
Caelo	Methadone hydrochloride	12344818	1
Caelo	Methadone hydrochloride	12344819	1
Caelo	Methadone hydrochloride	13266502	2
Caelo	Methadone hydrochloride	13266511	2
Caelo	Methadone hydrochloride	15244705	2
Caelo	Methadone hydrochloride	15244710	4
Caelo	Methadone hydrochloride	15244701	1
Caelo	Methadone hydrochloride	15244717	6
Caelo	Methadone hydrochloride	15244715	3
Caelo	Methadone hydrochloride	15244718	1
Caelo	Methadone hydrochloride	16135308	5
Caelo	Methadone hydrochloride	16135307	2
Caelo	Methadone hydrochloride	16135303	1
Caelo	Methadone hydrochloride	16135305	6
Caelo	Methadone hydrochloride	16135301	1
Caelo	Methadone hydrochloride	28041725	1
Caelo	Methadone hydrochloride	16135310	4
Caelo	Methadone hydrochloride	28061702	1
Caelo	Methadone hydrochloride	16135315	1
Caelo	Methadone hydrochloride	16135317	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Methadone hydrochloride	16135324	6
Caelo	Methadone hydrochloride	16135329	12
Caelo	Methadone hydrochloride	1613529	1
Caelo	Methadone hydrochloride	7091708	1
Caelo	Methadone hydrochloride	25111701	1
Caelo	Methadone hydrochloride	17239502	3
Caelo	Methadone hydrochloride	1729504	1
Caelo	Methadone hydrochloride	2912161	1
Caelo	Methadone hydrochloride	16135323	1
Caelo	Methadone hydrochloride	17239507	4
Caelo	Methadone hydrochloride	23021802	1
Caelo	Methadone hydrochloride	17239510	6
Caelo	Methadone hydrochloride	17239501	1
Caelo	Methadone hydrochloride	17051801	1
Caelo	Methadone hydrochloride	1723	1
Caelo	Methadone hydrochloride	17239518	6
Caelo	Methadone hydrochloride	17239514	1
Caelo	Methadone hydrochloride	1816601	1
Caelo	Methadone hydrochloride	18186601	12
Caelo	Methadone hydrochloride	1723509	1
Caelo	Methadone hydrochloride	177239518	1
Caelo	Methadone hydrochloride	3111806	1
Caelo	Methadone hydrochloride	18186608	11
Caelo	Methadone hydrochloride	19011913	1
Caelo	Methadone hydrochloride	31011901	1
Caelo	Methadone hydrochloride	18132406	4
Caelo	Methadone hydrochloride	18132413	11
Caelo	Methadone hydrochloride	18c01b05350572	1
Caelo	Methadone hydrochloride	18g02-b02-355992	1
Caelo	Methadone hydrochloride	18g02-b02355992	1
Caelo	Methadone hydrochloride	191494001	9
Caelo	Methadone hydrochloride	19149409	3
Caelo	Methadone hydrochloride	19000787001	9
Caelo	Methadone hydrochloride	19149404	1
Caelo	Methadone hydrochloride	21000271013	3
Caelo	Methadone hydrochloride	21003277011	2
Caelo	Methadone hydrochloride	21003277014	3
Caelo	Methadone hydrochloride	17239506	11
Caelo	Methadone hydrochloride	15244720	1
Caelo	Methadone hydrochloride	20170728/Ma2	1
Caelo	Methadone hydrochloride	19149407	2
Caelo	Methadone hydrochloride	15244713	4
Caelo	Methadone hydrochloride	191494003	12
Caelo	Methadone hydrochloride	19000787016	2
Caelo	Methadone hydrochloride	18186601P-181001-4	1
Caelo	Methadone hydrochloride	18132405P-190225-10	1
Caelo	Methadone hydrochloride	18132413P-190916-1	1
Caelo	Methadone hydrochloride	19149402P-191223-1	1
Caelo	Methadone hydrochloride	18132405P-190527-1	1
Caelo	Methadone hydrochloride	19000787001P2006221	1
Caelo	Methadone hydrochloride	19149406P-200323-2	1
Caelo	Methadone hydrochloride	18132413P-190709-2	1
Caelo	Methadone hydrochloride	21003277006	13
Caelo	Methadone hydrochloride	57(18132413)	1
Caelo	Methadone hydrochloride	61(19000787001)	1
Caelo	Methadone hydrochloride	14C24-B01-292860	2
Caelo	Methadone hydrochloride	M260813	1
Caelo	Methadone hydrochloride	11021904	1
Caelo	Methadone hydrochloride	18132408/	1
Caelo	Methadone hydrochloride	19000787002	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Methadone hydrochloride	18132408	17
Caelo	Methadone hydrochloride	1327H051	1
Caelo	Methadone hydrochloride	13266521	1
Caelo	Methadone hydrochloride	19149406	4
Caelo	Methadone hydrochloride	16135325	4
Caelo	Methadone hydrochloride	18132405	5
Caelo	Methadone hydrochloride	19000824003	1
Caelo	Methadone hydrochloride	19149403	1
Caelo	Methadone hydrochloride	190603141F	1
Caelo	Methadone hydrochloride	13266515	1
Caelo	Methadone hydrochloride	16135327	12
Caelo	Methadone hydrochloride	16135322	1
Caelo	Methadone hydrochloride	17I15-B02-339523	8
Caelo	Methadone hydrochloride	17239512	12
Caelo	Methadone hydrochloride	58(18132417)	1
Caelo	Methadone hydrochloride	21000271007	4
Caelo	Methadone hydrochloride	21003277009	7
Caelo	Methadone hydrochloride	16135302	1
Caelo	Methadone hydrochloride	16135318	8
Caelo	Methadone hydrochloride	16135326	11
Caelo	Methadone hydrochloride	16135325,170814MHC	1
Caelo	Methadone hydrochloride	16135332	11
Caelo	Methadone hydrochloride	172329504	1
Caelo	Methadone hydrochloride	16135328	1
Caelo	Methadone hydrochloride	180219MC/17239506	1
Caelo	Methadone hydrochloride	17239503	4
Caelo	Methadone hydrochloride	19149402	9
Caelo	Methadone hydrochloride	19D09-B03-3645508	1
Caelo	Methadone hydrochloride	21000271001	1
Caelo	Methadone hydrochloride	21003277001	1
Caelo	Methadone hydrochloride	12344802	1
Caelo	Methadone hydrochloride	15244709	2
Caelo	Methadone hydrochloride	16135330	5
Caelo	Methadone hydrochloride	171920-0004	1
Caelo	Methadone hydrochloride	18132412	11
Caelo	Methadone hydrochloride	13266514	1
Caelo	Methadone hydrochloride	15I24-B07-317266	1
Caelo	Methadone hydrochloride	16F24-B02-323184	1
Caelo	Methadone hydrochloride	18132409	1
Caelo	Methadone hydrochloride	190000787013	1
Caelo	Methadone hydrochloride	21000271004	2
Caelo	Methadone hydrochloride	220901smi//21000271019	1
Caelo	Methadone hydrochloride	LOT067055	1
Caelo	Methadone hydrochloride	70925	1
Caelo	Methadone hydrochloride	12171906	2
Caelo	Methadone hydrochloride	12344816	3
Caelo	Methadone hydrochloride	13266501	1
Caelo	Methadone hydrochloride	13266505	4
Caelo	Methadone hydrochloride	13266518	3
Caelo	Methadone hydrochloride	15215501	1
Caelo	Methadone hydrochloride	15244704	4
Caelo	Methadone hydrochloride	15244706	3
Caelo	Methadone hydrochloride	16208016	1
Caelo	Methadone hydrochloride	17239508	3
Caelo	Methadone hydrochloride	18186604	4
Caelo	Methadone hydrochloride	18132404	3
Caelo	Methadone hydrochloride	21000271019	7
Caesar & Loretz GmbH	Methadone hydrochloride	18186607	5
Caesar & Loretz GmbH	Methadone hydrochloride	18132407	3
Caesar & Loretz GmbH	Methadone hydrochloride	18132417	13

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caesar & Loretz GmbH	Methadone hydrochloride	18186605	1
Caesar & Loretz GmbH	Methadone hydrochloride	18132416	4
Caesar & Loretz GmbH	Methadone hydrochloride	19000787003	6
Caesar & Loretz GmbH	Methadone hydrochloride	19000824004	3
Caesar & Loretz GmbH	Methadone hydrochloride	19000787005	3
Caesar & Loretz GmbH	Methadone hydrochloride	20D09-F05-371481	1
Caesar & Loretz GmbH	Methadone hydrochloride	21000271002	4
Caesar & Loretz GmbH	Methadone hydrochloride	19000787013	2
Caesar & Loretz GmbH	Methadone hydrochloride	21000271009	4
Caesar & Loretz GmbH	Methadone hydrochloride	f05-3714801	1
Caesar & Loretz GmbH	Methadone hydrochloride	F01-3764906	2
Caesar & Loretz GmbH	Methadone hydrochloride	21000271011	5
Caesar & Loretz GmbH	Methadone hydrochloride	21000271012	1
Caesar & Loretz GmbH	Methadone hydrochloride	21000271017	3
Caesar & Loretz GmbH	Methadone hydrochloride	21000271010	1
Caesar & Loretz GmbH	Methadone hydrochloride	21003277015	1
Caesar & Loretz GmbH	Methadone hydrochloride	21003277010	1
Caesar & Loretz GmbH/	Methadone hydrochloride	191494	2
Caesar & Loretz Gm…	Methadone hydrochloride	19000787012	2
Caesar & Loretz Gm…	Methadone hydrochloride	18186603	2
Caesar & Loretz Gm…	Methadone hydrochloride	19149405	1
Caesar & Loretz Gm…	Methadone hydrochloride	19000787004	5
Cordes/Alia	Methadone hydrochloride	19000787008	9
Dr. Wolff	Methadone hydrochloride	16F24-B02	1
Ebert-Jacobi	Methadone hydrochloride	16135306	1
Euro OTC	Methadone hydrochloride	14C24-B01	2
Fagron	Methadone hydrochloride	21G14-F06-379152	2
Faagron	Methadone hydrochloride	1437H011	1
Fagro/ Noweda	Methadone hydrochloride	17/15-B02-339527	1
Fagro//Noweda	Methadone hydrochloride	15/24-B07-317267	1
Fagro/Jenne	Methadone hydrochloride	17I15-B02-339525	2
Fagron	Methadone hydrochloride	12B21N03	1
Fagron	Methadone hydrochloride	11G11-N02	1
Fagron	Methadone hydrochloride	17115-B02-339521	1
Fagron	Methadone hydrochloride	12H07-N07	1
Fagron	Methadone hydrochloride	20130912-6	1
Fagron	Methadone hydrochloride	12H07-N05	4
Fagron	Methadone hydrochloride	1213E-02949	1
Fagron	Methadone hydrochloride	9041306	1
Fagron	Methadone hydrochloride	171920-0009	1
Fagron	Methadone hydrochloride	1225H008	1
Fagron	Methadone hydrochloride	13B06-N02	5
Fagron	Methadone hydrochloride	13F17-N02	6
Fagron	Methadone hydrochloride	25091307	1
Fagron	Methadone hydrochloride	414022-1-P	1
Fagron	Methadone hydrochloride	11D07-N09	1
Fagron	Methadone hydrochloride	13I24-B06-286908	1
Fagron	Methadone hydrochloride	25091406	1
Fagron	Methadone hydrochloride	13J24-B06-286907	1
Fagron	Methadone hydrochloride	1327h051	1
Fagron	Methadone hydrochloride	14C24-B01-292857	4
Fagron	Methadone hydrochloride	4031517	1
Fagron	Methadone hydrochloride	14H15-B01-299381	1
Fagron	Methadone hydrochloride	29051502	1
Fagron	Methadone hydrochloride	15B24-B02-304724	6
Fagron	Methadone hydrochloride	8081501	1
Fagron	Methadone hydrochloride	1437H012	2
Fagron	Methadone hydrochloride	13J24-B06-286906	1
Fagron	Methadone hydrochloride	15E29-B02-313031	1
Fagron	Methadone hydrochloride	13J24B06286910	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Methadone hydrochloride	1514H042	3
Fagron	Methadone hydrochloride	2877	1
Fagron	Methadone hydrochloride	1608H002	3
Fagron	Methadone hydrochloride	16F24-B02-323185	1
Fagron	Methadone hydrochloride	16K01-B04-329933	3
Fagron	Methadone hydrochloride	16K01B04	1
Fagron	Methadone hydrochloride	16K01-B04-329934	2
Fagron	Methadone hydrochloride	16K01-B04	2
Fagron	Methadone hydrochloride	17C24-B05-334309	6
Fagron	Methadone hydrochloride	16-k01-B04-329937	1
Fagron	Methadone hydrochloride	17I15-B02-339529	2
Fagron	Methadone hydrochloride	17c24b05334309	1
Fagron	Methadone hydrochloride	17I15-B02-339521	6
Fagron	Methadone hydrochloride	17/15-B02-339521	4
Fagron	Methadone hydrochloride	15/24-B07-313517	1
Fagron	Methadone hydrochloride	17|15-B02-339521	1
Fagron	Methadone hydrochloride	17I15-B02-343153	1
Fagron	Methadone hydrochloride	17l15-B02-343153	1
Fagron	Methadone hydrochloride	339527	1
Fagron	Methadone hydrochloride	17/15-B02-343153	1
Fagron	Methadone hydrochloride	17105-B02	1
Fagron	Methadone hydrochloride	18G02-B02	7
Fagron	Methadone hydrochloride	18G02B02351285	2
Fagron	Methadone hydrochloride	1801h11	1
Fagron	Methadone hydrochloride	17I15-B02-343150	5
Fagron	Methadone hydrochloride	1801h011	1
Fagron	Methadone hydrochloride	18G02-B02-355993	2
Fagron	Methadone hydrochloride	18G02-B02-355994	1
Fagron	Methadone hydrochloride	18c01-b05-350572	1
Fagron	Methadone hydrochloride	18gb02-35599202-	1
Fagron	Methadone hydrochloride	16K01-B04-329936	1
Fagron	Methadone hydrochloride	17I15-B02-339528	1
Fagron	Methadone hydrochloride	19D09-B03-364518	1
Fagron	Methadone hydrochloride	17/15-B02-343150	1
Fagron	Methadone hydrochloride	19D09-B03-364519	1
Fagron	Methadone hydrochloride	19D09-B03-364516	2
Fagron	Methadone hydrochloride	18C01-B05-350572	1
Fagron	Methadone hydrochloride	19D09-B03_364513	1
Fagron	Methadone hydrochloride	1914H016	3
Fagron	Methadone hydrochloride	20D09F05	3
Fagron	Methadone hydrochloride	20A09-F05	5
Fagron	Methadone hydrochloride	20A09-F05-370759	1
Fagron	Methadone hydrochloride	20A09-F05-370755	5
Fagron	Methadone hydrochloride	21A06-F01-376497	2
Fagron	Methadone hydrochloride	21A06-F01	3
Fagron	Methadone hydrochloride	21G14-F06	2
Fagron	Methadone hydrochloride	21A06-F01-376496	1
Fagron	Methadone hydrochloride	1814H016	1
Fagron	Methadone hydrochloride	2117H030	3
Fagron	Methadone hydrochloride	21G14-F06-379151	1
Fagron	Methadone hydrochloride	21H25-F02-380956	1
Fagron	Methadone hydrochloride	13J24-B06-286908	1
Fagron	Methadone hydrochloride	F04-3825003	1
Fagron	Methadone hydrochloride	21H25-F02-380953	1
Fagron	Methadone hydrochloride	1409H043	1
Fagron	Methadone hydrochloride	18C01-B05-346737	7
Fagron	Methadone hydrochloride	18C01-B05-350573	2
Fagron	Methadone hydrochloride	19D09-B03	7
Fagron	Methadone hydrochloride	20D09-F05-370590	1
Fagron	Methadone hydrochloride	20A09-F05-370758	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Methadone hydrochloride	21G14-F06-379154	1
Fagron	Methadone hydrochloride	21H25-F02-380954	1
Fagron	Methadone hydrochloride	21H25-F02-380291	2
Fagron	Methadone hydrochloride	15E29-B02-313098	3
Fagron	Methadone hydrochloride	15B24-B02-313097	1
Fagron	Methadone hydrochloride	17c24-bo5334311	1
Fagron	Methadone hydrochloride	17115-B02-343154	2
Fagron	Methadone hydrochloride	20D09-F05-371480	1
Fagron	Methadone hydrochloride	15E29_B02_309070	1
Fagron	Methadone hydrochloride	1316H037	4
Fagron	Methadone hydrochloride	17115-B02	1
Fagron	Methadone hydrochloride	17C24-B05-335712	1
Fagron	Methadone hydrochloride	1715-B02-343151	1
Fagron	Methadone hydrochloride	211BH003	1
Fagron	Methadone hydrochloride	15I24-B07	1
Fagron	Methadone hydrochloride	16F24-B02-323186	1
Fagron	Methadone hydrochloride	17C24-B05-334311	2
Fagron	Methadone hydrochloride	18G02-B02-351285	1
Fagron	Methadone hydrochloride	19149401	3
Fagron	Methadone hydrochloride	19D09-B03-364517	4
Fagron	Methadone hydrochloride	20D09-F05-370589	4
Fagron	Methadone hydrochloride	19D09-B03-364560	1
Fagron	Methadone hydrochloride	20A09-F05-370757	2
Fagron	Methadone hydrochloride	21A06-F02-376492	3
Fagron	Methadone hydrochloride	21A06-F02	1
Fagron	Methadone hydrochloride	16f24-b02-323184	1
Fagron	Methadone hydrochloride	17C24-B05-335711	11
Fagron	Methadone hydrochloride	17I15W02	1
Fagron	Methadone hydrochloride	350571	1
Fagron	Methadone hydrochloride	21002144002	1
Fagron	Methadone hydrochloride	16k01-b04-329933	1
Fagron	Methadone hydrochloride	12A05-No2	1
Fagron	Methadone hydrochloride	14H15-B01-299382	6
Fagron	Methadone hydrochloride	15E29-B02-309070	2
Fagron	Methadone hydrochloride	1715-B02-339523	1
Fagron	Methadone hydrochloride	18C01-B05-350571	11
Fagron	Methadone hydrochloride	19D09-B03-364514	3
Fagron	Methadone hydrochloride	19D9-B03-364514	1
Fagron	Methadone hydrochloride	16F24-B02-323182	1
Fagron	Methadone hydrochloride	16F24-B02-326207	3
Fagron	Methadone hydrochloride	170427MH/1608H002	1
Fagron	Methadone hydrochloride	16F24-B02-329935	1
Fagron	Methadone hydrochloride	1801H011	3
Fagron	Methadone hydrochloride	18G02-B02-355991	1
Fagron	Methadone hydrochloride	1847H015	6
Fagron	Methadone hydrochloride	19D09-B03_364514	1
Fagron	Methadone hydrochloride	14H15-B01	1
Fagron	Methadone hydrochloride	17C24-B-335711	1
Fagron	Methadone hydrochloride	20A09F05	1
Fagron	Methadone hydrochloride	19D09-B03-364558	4
Fagron	Methadone hydrochloride	B03-3645508	1
Fagron	Methadone hydrochloride	1718H028	14
Fagron	Methadone hydrochloride	1718HO28	1
Fagron	Methadone hydrochloride	17/15-B02	1
Fagron	Methadone hydrochloride	19D09-B03-364559	1
Fagron	Methadone hydrochloride	200000000	1
Fagron	Methadone hydrochloride	1207h057	1
Fagron	Methadone hydrochloride	F05-3714709	2
Fagron	Methadone hydrochloride	20D09-F05	3
Fagron	Methadone hydrochloride	F05-3705809	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Methadone hydrochloride	22E02-F04-382503	3
Fagron	Methadone hydrochloride	12b21-n03	1
Fagron	Methadone hydrochloride	16B16-B02-318420	3
Fagron	Methadone hydrochloride	17I15-B02	8
Fagron	Methadone hydrochloride	1715-B02-339525	2
Fagron	Methadone hydrochloride	15-B02-339525	1
Fagron	Methadone hydrochloride	1715-B02-343150	1
Fagron	Methadone hydrochloride	15-B02-343150	1
Fagron	Methadone hydrochloride	18G02-B02-355990	8
Fagron	Methadone hydrochloride	19D09-B03-364513	10
Fagron	Methadone hydrochloride	21H25-F02	2
Fagron	Methadone hydrochloride	18G02-B02-35590	1
Fagron	Methadone hydrochloride	20A09-F05-371479	1
Fargon	Methadone hydrochloride	16K01-B04-329937	2
Gatt-Koller	Methadone hydrochloride	1801702	1
gehe	Methadone hydrochloride	16135316	4
Gehe	Methadone hydrochloride	17115-B02-339523	1
Gehe	Methadone hydrochloride	23001353007	1
Caelo	Methadone hydrochloride	21003277005	1
Gehe/Noweda	Methadone hydrochloride	16135319	3
Hedinger/ Sanacorp	Methadone hydrochloride	15215505	3
Jenne	Methadone hydrochloride	15B24-B02	1
Klosterring	Methadone hydrochloride	17I15-B02-343151	4
L30	Methadone hydrochloride	67055	26
NOW	Methadone hydrochloride	23A25-F-02-384693	1
noweda	Methadone hydrochloride	3072001	1
Noweda	Methadone hydrochloride	20a09f05370755	1
Noweda	Methadone hydrochloride	23001353005	1
Fagron	Methadone hydrochloride	17c24-b05	1
Caelo	Methadone hydrochloride	12171918	1
Caelo	Methadone hydrochloride	12344812	2
Caelo	Methadone hydrochloride	12344807	1
Caelo	Methadone hydrochloride	12344814	2
Caelo	Methadone hydrochloride	13266504	2
Caelo	Methadone hydrochloride	17C24-B05	2
Euro OTC	Methadone hydrochloride	16135304	5
Phoenix	Methadone hydrochloride	16125317	1
Phönix	Methadone hydrochloride	16135309	3
Phönix	Methadone hydrochloride	2100327706	1
Caelo	Methadone hydrochloride	17239504	8
Fagron	Methadone hydrochloride	16F24B02323184	2
Sanacorp	Methadone hydrochloride	12171913	1
Sanacorp	Methadone hydrochloride	12344806	2
Siegfried Ltd	Methadone hydrochloride	12B21-N03	1
Siegfried Ltd, Div…	Methadone hydrochloride	15244712	1
Fagron	Methadone hydrochloride	F05-3707509	3
Fagron	Methadone hydrochloride	F01-3764907	1
Siegfried Ltd. Dev…	Methadone hydrochloride	17186104	1
Th. Geyer	Methadone hydrochloride	70873	1
Th. Geyer	Methadone hydrochloride		2
Th. Geyer	Methadone hydrochloride	67047	2
Th. Geyer	Methadone hydrochloride	56(070245)	1
Th. Geyer	Methadone hydrochloride	70245	86
Th. Geyer	Methadone hydrochloride	70246	1
VDL;87,00EUR;08.09.14	Methadone hydrochloride	12344821	1
ZL	Methadone hydrochloride	70617	19
Caelo	Methylrosanilinium chloride	9238107	1
Caelo	Methylrosanilinium chloride	12H28-N06	1
Caelo	Methylrosanilinium chloride	3455360	1
Caelo	Methylrosanilinium chloride	13184801	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Methylrosanilinium chloride	12H28-No6	1
Caelo	Methylrosanilinium chloride	9238109	1
Caelo	Methylrosanilinium chloride	9238106	1
Fagron	Methylrosanilinium chloride	12H28_N06	1
Fagron	Methylrosanilinium chloride	13H28-N03	2
Fagron	Methylrosanilinium chloride	1989	2
Fagron	Methylrosanilinium chloride	13G03N11	1
Fagron	Methylrosanilinium chloride	13H28-No3	1
Fagron	Methylrosanilinium chloride	13G03-N011	1
Fagron	Methylrosanilinium chloride	13G03-N11	1
Fagron	Methylrosanilinium chloride	13H28-N03	18
Fagron	Methylrosanilinium chloride	13H28-N03-0161-1030	1
Fagron	Methylrosanilinium chloride	12-17-N050109-140	1
Fagron	Methylrosanilinium chloride	12D19-N01	1
Fagron	Methylrosanilinium chloride	13H28-NO3	1
Fagron	Methylrosanilinium chloride	13G03-N11	1
Fagron	Methylrosanilinium chloride	12I17-N05	1
Noweda	Methylrosanilinium chloride	9238104	1
Noweda	Methylrosanilinium chloride	12H28-NO6	1
Noweda	Methylrosanilinium chloride	2159	2
Caelo	Methylrosanilinium chloride	12/17-N05	1
phönix	Methylrosanilinium chloride	13184811	1
Fagron	Midazolam	14C12-B31-313222	1
Fagron	Midazolam	16J03-B09-326963	1
	Midazolam hydrochloride	21B03-F50-384281	3
	Midazolam hydrochloride	20002613005	1
	Midazolam hydrochloride	21B03	1
	Midazolam hydrochloride	24B16-F02-386032	1
Caelo	Midazolam hydrochloride	2061508	1
Caelo	Midazolam hydrochloride	15224603	1
Caelo	Midazolam hydrochloride	15224607	2
Caelo	Midazolam hydrochloride	15224614	2
Caelo	Midazolam hydrochloride	14339002	1
Caelo	Midazolam hydrochloride	15224616	3
Caelo	Midazolam hydrochloride	16290605	10
Caelo	Midazolam hydrochloride	17168001	1
Caelo	Midazolam hydrochloride	17168009	4
Caelo	Midazolam hydrochloride	192213002	5
Caelo	Midazolam hydrochloride	11184705	1
Caelo	Midazolam hydrochloride	17168005	1
Caelo	Midazolam hydrochloride	143339009	1
Caelo	Midazolam hydrochloride	20002613002	6
Caelo	Midazolam hydrochloride	2100053006	1
Caelo	Midazolam hydrochloride	15224605	1
Caelo	Midazolam hydrochloride	14339009	1
Caelo	Midazolam hydrochloride	83600116001	1
Caelo	Midazolam hydrochloride	14339015	2
Caelo	Midazolam hydrochloride	17168006	7
Caelo	Midazolam hydrochloride	71680091	1
Caelo	Midazolam hydrochloride	20002613004	2
Caesar & Loretz GmbH	Midazolam hydrochloride	20002613009	1
Caesar & Loretz GmbH	Midazolam hydrochloride	21000038007	4
Caesar & Loretz GmbH	Midazolam hydrochloride	21000535006	2
Caesar & Loretz GmbH	Midazolam hydrochloride	20002613010	1
Caesar & Loretz GmbH	Midazolam hydrochloride	21003167002	11
Caesar & Loretz GmbH	Midazolam hydrochloride	21003167008	2
Caesar & Loretz GmbH	Midazolam hydrochloride	21003167004	1
Caesar & Loretz Gm…	Midazolam hydrochloride	2100003807	1
Caesar & Loretz Gm…	Midazolam hydrochloride	21000038005	1
Caesar & Loretz Gm…	Midazolam hydrochloride	17168007	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Eurho/Phoenix	Midazolam hydrochloride	12L17-N10	1
Fagron	Midazolam hydrochloride	9D27-N01	2
Fagron	Midazolam hydrochloride	11A31-NO1	1
Fagron	Midazolam hydrochloride	15H04-B03-314396	9
Fagron	Midazolam hydrochloride	400101	1
Fagron	Midazolam hydrochloride	940112	2
Fagron	Midazolam hydrochloride	18B28-B05-354856	2
Fagron	Midazolam hydrochloride	17K21-B05-347538	2
Fagron	Midazolam hydrochloride	18F19-B02	1
Fagron	Midazolam hydrochloride	18F19-B02-354857	4
Fagron	Midazolam hydrochloride	18F19B02	1
Fagron	Midazolam hydrochloride	20D21-F02	1
Fagron	Midazolam hydrochloride	20D21-F02-370326	2
Fagron	Midazolam hydrochloride	14H05-B08-297982	1
Fagron	Midazolam hydrochloride	20F11-F04-374727	1
Fagron	Midazolam hydrochloride	20I24-F01	3
Fagron	Midazolam hydrochloride	18F19B02-354857	1
Fagron	Midazolam hydrochloride	20I24-F01-374730	3
Fagron	Midazolam hydrochloride	16C14-B12-332469	1
Fagron	Midazolam hydrochloride	18B28-B05	2
Fagron	Midazolam hydrochloride	19I25-F03-365483	1
Fagron	Midazolam hydrochloride	20D21-F02-370327	1
Fagron	Midazolam hydrochloride	F01-3747208	2
Fagron	Midazolam hydrochloride	30916	1
Fagron	Midazolam hydrochloride	20124-F01-374730	1
Fagron	Midazolam hydrochloride	20I24-F01-374728	7
JENNE	Midazolam hydrochloride	17168003	5
Noweda	Midazolam hydrochloride	17168011	5
Noweda	Midazolam hydrochloride	2100003805	1
Anzag ek:2,64EUR 16.07.12	Mistletoe	10273417	1
Aurica/Phönix	Mistletoe	6110801	1
Bombastus	Mistletoe	277432	2
Caelo	Mistletoe	29061201	1
Caelo	Mistletoe	10273412	1
Caelo	Mistletoe	10081205	1
Caelo	Mistletoe	10091201	1
Caelo	Mistletoe	11294003	2
Caelo	Mistletoe	23111204	1
Caelo	Mistletoe	10273418	1
Caelo	Mistletoe	10273420	5
Caelo	Mistletoe	12011301	1
Caelo	Mistletoe	11266704	14
Caelo	Mistletoe	11021303	1
Caelo	Mistletoe	11266708	8
Caelo	Mistletoe	11266705	3
Caelo	Mistletoe	18031303	1
Caelo	Mistletoe	11266710	7
Caelo	Mistletoe	6061306	1
Caelo	Mistletoe	17061304	1
Caelo	Mistletoe	26071302	1
Caelo	Mistletoe	29071302	1
Caelo	Mistletoe	29081302	1
Caelo	Mistletoe	28101304	1
Caelo	Mistletoe	29101302	1
Caelo	Mistletoe	20121303	1
Caelo	Mistletoe	27121305	1
Caelo	Mistletoe	24011401	1
Caelo	Mistletoe	14292506	2
Caelo	Mistletoe	14292514	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Mistletoe	11266714	4
Caelo	Mistletoe	11266703	3
Caelo	Mistletoe	11266712-3450311162	1
Caelo	Mistletoe	11266702	4
Caelo	Mistletoe	10273407	1
Caelo	Mistletoe	11294004	5
Caelo	Mistletoe	3813E-01695	1
Caelo	Mistletoe	4313E-01695	1
Caelo	Mistletoe	11266713	2
Galke	Mistletoe	20328	1
Galke	Mistletoe	22012	2
Gesundform	Mistletoe	216482	1
Haustee	Mistletoe	57010507	1
Caelo	Mistletoe	11294005	15
Klenk	Mistletoe	4691A120507	2
Klenk	Mistletoe	4691A110816	2
Klenk	Mistletoe	1512211695	1
Klenk	Mistletoe	2901311695	1
Klenk	Mistletoe	110816	1
Klenk	Mistletoe	4691A130307	7
Klenk	Mistletoe	4691A121122	11
Klenk	Mistletoe	4961A120419	1
Klenk	Mistletoe	4691a130307	1
Klenk	Mistletoe	4691A-120507	1
Klenk	Mistletoe	4691a121122	1
Klenk	Mistletoe	4691A121122-35454110	1
Noweda	Mistletoe	11294001	1
Caelo	Mistletoe	11266709	10
Caelo	Mistletoe	11266712	8
Klenk	Mistletoe	4691A120419	6
Spangropharm	Mistletoe	10273408	1
Caelo	Molecular distilled glycero…	11160012	1
Noweda	Molecular distilled glycero…	11160010	1
	Morphine hydrochloride	20003757015	1
	Morphine hydrochloride	21002337009	1
	Morphine hydrochloride	23003282004	2
04655198	Morphine hydrochloride	2003757008	1
Caelo	Morphine hydrochloride	12318101	1
Caelo	Morphine hydrochloride	13081310	1
Caelo	Morphine hydrochloride	12104409	1
Caelo	Morphine hydrochloride	14238604	1
Caelo	Morphine hydrochloride	15199705	1
Caelo	Morphine hydrochloride	15199705Nr.2	1
Caelo	Morphine hydrochloride	15199705Nr.3	1
Caelo	Morphine hydrochloride	15199711	4
Caelo	Morphine hydrochloride	14238619	2
Caelo	Morphine hydrochloride	15199709	1
Caelo	Morphine hydrochloride	1543904	1
Caelo	Morphine hydrochloride	15439409	1
Caelo	Morphine hydrochloride	15439406	3
Caelo	Morphine hydrochloride	13125208	1
Caelo	Morphine hydrochloride	15439405	2
Caelo	Morphine hydrochloride	15439402	1
Caelo	Morphine hydrochloride	16184602	2
Caelo	Morphine hydrochloride	16184605	2
Caelo	Morphine hydrochloride	14081701	1
Caelo	Morphine hydrochloride	16184610	2
Caelo	Morphine hydrochloride	16184609	2
Caelo	Morphine hydrochloride	15199707	1
Caelo	Morphine hydrochloride	16184614	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Morphine hydrochloride	16184607	1
Caelo	Morphine hydrochloride	18188603	3
Caelo	Morphine hydrochloride	118188607	2
Caelo	Morphine hydrochloride	18188611	2
Caelo	Morphine hydrochloride	48188601	1
Caelo	Morphine hydrochloride	18188612	3
Caelo	Morphine hydrochloride	193085002	3
Caelo	Morphine hydrochloride	193085007	9
Caelo	Morphine hydrochloride	193085009	1
Caelo	Morphine hydrochloride	193085012	1
Caelo	Morphine hydrochloride	20001998002	2
Caelo	Morphine hydrochloride	20003757003	2
Caelo	Morphine hydrochloride	20003757010	3
Caelo	Morphine hydrochloride	1818866	1
Caelo	Morphine hydrochloride	16184613	7
Caelo	Morphine hydrochloride	18188602	2
Caelo	Morphine hydrochloride	12104403	1
Caelo	Morphine hydrochloride	15439413	2
Caelo	Morphine hydrochloride	17258002NR:51/18	1
Caelo	Morphine hydrochloride	14055084	1
Caelo	Morphine hydrochloride	193085008	1
Caelo	Morphine hydrochloride	18188614	6
Caelo	Morphine hydrochloride	193085014	2
Caelo	Morphine hydrochloride	13125206	1
Caelo	Morphine hydrochloride	15199713	1
Caelo	Morphine hydrochloride	17258002	6
Caelo	Morphine hydrochloride	18188606	5
Caesar & Loretz GmbH	Morphine hydrochloride	15199711(1)	1
Caesar & Loretz GmbH	Morphine hydrochloride	15199711(2)	1
Caesar & Loretz GmbH	Morphine hydrochloride	15199712	1
Caesar & Loretz GmbH	Morphine hydrochloride	15199711	1
Caesar & Loretz GmbH	Morphine hydrochloride	18188607	1
Caesar & Loretz GmbH	Morphine hydrochloride	18188610	2
Caesar & Loretz GmbH	Morphine hydrochloride	18188617	2
Caesar & Loretz GmbH	Morphine hydrochloride	18188613	3
Caesar & Loretz GmbH	Morphine hydrochloride	193085003	3
Caesar & Loretz GmbH	Morphine hydrochloride	193085006	4
Caesar & Loretz GmbH	Morphine hydrochloride	20003757001	4
Caesar & Loretz GmbH	Morphine hydrochloride	193085005	1
Caesar & Loretz GmbH	Morphine hydrochloride	20003757004	9
Caesar & Loretz GmbH	Morphine hydrochloride	20003757002	2
Caesar & Loretz GmbH	Morphine hydrochloride	20003757006	1
Caesar & Loretz Gm...	Morphine hydrochloride	20003757008	2
Fagron	Morphine hydrochloride	11A27-N04	1
Fagron	Morphine hydrochloride	12E10N04	1
Fagron	Morphine hydrochloride	13D09-N04	1
Fagron	Morphine hydrochloride	15A12-B04-303137	1
Fagron	Morphine hydrochloride	15J27_B01_316889	1
Fagron	Morphine hydrochloride	16D21-B02-322087	1
Fagron	Morphine hydrochloride	17F22-B01-338170	2
Fagron	Morphine hydrochloride	18F11-B03-361065	1
Fagron	Morphine hydrochloride	20E28-F06	1
Fagron	Morphine hydrochloride	18B26-B04-351286	1
Fagron	Morphine hydrochloride	20E28-F06-372132	3
Fagron	Morphine hydrochloride	12E10-N04	2
Fagron	Morphine hydrochloride	17C24-B03-334287	1
Fagron	Morphine hydrochloride	15/09-B08-312693	1
Fagron	Morphine hydrochloride	15I09-B08-312693	2
Fagron	Morphine hydrochloride	B02-3220808	1
Fagron	Morphine hydrochloride	13H22-N12	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Th. Geyer	Morphine hydrochloride	PH120087	1
Th. Geyer	Morphine hydrochloride	1415E-01879	1
Th. Geyer	Morphine hydrochloride	2615M-01879	1
Jenne	Morphine hydrochloride	20001998001	1
Phoenix	Morphine hydrochloride	18F11-B03-357051	2
Caelo	Morphine hydrochloride	14238617	1
Phönix	Morphine hydrochloride	18188601	4
Sanacorp	Morphine hydrochloride	16184612	2
Sanacorp	Morphine hydrochloride	21002337005	3
Caelo	Morphine hydrochloride	15439411	1
Synop	Morphine hydrochloride	15I09-B08	1
Th. Geyer	Morphine hydrochloride	4117A-01879	1
Th. Geyer	Morphine hydrochloride	3518M-01879	1
Th. Geyer	Morphine hydrochloride	67036	5
Caelo	Morphine sulfate	17331507	1
Caelo	Morphine sulfate	17331510	4
Caelo	Motherwort	5061203	1
Caelo	Motherwort	12376403	1
Caelo	Motherwort	12376408	2
Caelo	Motherwort	12376407	1
Caelo	Motherwort	11293004	1
Gehe	Motherwort	12231502	3
Klenk	Motherwort	4071A-100707	1
Phönix	Motherwort	12231503	2
Caelo	Mullein flower, cut	12317104	1
Caelo	Mullein flower, cut	521505390	1
Caelo	Mullein flower, cut	11020802	2
Caelo	Mullein flower, cut	11020902	1
Caelo	Mullein flower, cut	16081201	1
Caelo	Mullein flower, cut	11020714	4
Caelo	Mullein flower, cut	11233401	4
Caelo	Mullein flower, cut	11366402	1
Caelo	Mullein flower, cut	12192901	3
Caelo	Mullein flower, cut	12192903	3
Caelo	Mullein flower, cut	18031301	1
Caelo	Mullein flower, cut	11233402	1
Caelo	Mullein flower, cut	11333402	1
Caelo	Mullein flower, cut	12170901	1
Caelo	Mullein flower, cut	12192904	1
Caelo	Mullein flower, cut	12192907	3
Caelo	Mullein flower, cut	13229702	1
Caelo	Mullein flower, cut	11020713	2
Caelo	Mullein flower, cut	1219203	1
Caelo	Mullein flower, cut	12192905	5
Caelo	Mullein flower, cut	11366403	1
Caelo	Mullein flower, cut	12170906	1
Caelo	Mullein flower, cut	13229701	2
Caesar/Noweda	Mullein flower, cut	2810E-01475	1
Hepart AG	Mullein flower, cut	12170904	2
Klenk	Mullein flower, cut	1650A100608	1
Klenk	Mullein flower, cut	1651B110203	2
Klenk	Mullein flower, cut	1650A111018	3
Klenk	Mullein flower, cut	A120612	1
Klenk	Mullein flower, cut	1650A120612	1
Klenk	Mullein flower, cut	1651B140324	2
Klenk	Mullein flower, cut	1651B150722	1
Klenk	Mullein flower, cut	1651B130820	5
Klenk	Mullein flower, cut	1651b130820	2
Klenk	Mullein flower, cut	1651B121109	22
Klenk	Mullein flower, cut	1651B120315	3

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Myrrh	11276810	1
Caelo	Myrrh	11276806	1
Caelo	Myrrh	11277111	1
Caelo	Myrrh	12269901	2
Caelo	Myrrh	12269907	1
Caelo	Myrrh	25071404	1
Caelo	Myrrh	28101401	1
Caelo	Myrrh	30121413	1
Caelo	Myrrh	12269913	1
Caelo	Myrrh	14347509	1
Caelo	Myrrh	15021410	1
Caelo	Myrrh	15312606	1
Caelo	Myrrh	12269904	4
Caelo	Myrrh	14244602	1
Caelo	Myrrh	11277111	1
Caelo	Myrrh	12244404	1
Caelo	Myrrh	12244406	1
Caelo	Myrrh	11277105	1
Caelo	Myrrh	13108701	2
Caelo	Myrrh	15021402	1
Klenk	Myrrh	3351A121004	1
Klenk	Myrrh	3351A130902	1
Klenk	Myrrh	3351A120514	1
Klenk	Myrrh	3355B140723	1
Klenk	Myrrh	3355B161010	1
Klenk	Myrrh	3351A160330	4
phönix	Myrrh	15021411	1
phönix	Myrrh	3351a160330	1

N

Supplier	Substance	Batch	Spectra
Anzag	Nettle leaf	2381-A130122	1
Anzag EK4,31 17.08.12	Nettle leaf	2381A110913	19
Klenk	Nettle leaf	2381a120619	4
Bahnhof-Apotheke	Nettle leaf	7-121109	1
Bombastus	Nettle leaf	266638	1
Bombastus	Nettle leaf	270987	3
Bombastus	Nettle leaf	270854	3
Bombastus	Nettle leaf	273229	2
Bombastus	Nettle leaf	275848	3
Bombastus	Nettle leaf	280305	2
Bombastus	Nettle leaf	276407	2
Bombastus	Nettle leaf	266099	1
Bombastus	Nettle leaf	275763	1
Caelo	Nettle leaf	12183908	5
Caelo	Nettle leaf	10291405	2
Caelo	Nettle leaf	10282807	2
Caelo	Nettle leaf	10282806	1
Caelo	Nettle leaf		3
Caelo	Nettle leaf	18071202	1
Caelo	Nettle leaf	10291413	1
Caelo	Nettle leaf	120375901	1
Caelo	Nettle leaf	10291411	2
Caelo	Nettle leaf	12195101	3
Caelo	Nettle leaf	17121205	1
Caelo	Nettle leaf	12184503	3
Caelo	Nettle leaf	10375901	2
Caelo	Nettle leaf	12184702	2
Caelo	Nettle leaf	7031302	1
Caelo	Nettle leaf	12184706	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Nettle leaf	12184001	6
Caelo	Nettle leaf	2051302	1
Caelo	Nettle leaf	12814001	1
Caelo	Nettle leaf	29071303	1
Caelo	Nettle leaf	intch:313011	1
Caelo	Nettle leaf	12183901	2
Caelo	Nettle leaf	1283910	1
Caelo	Nettle leaf	13091302	1
Caelo	Nettle leaf	12183911	16
Caelo	Nettle leaf	12183909	1
Caelo	Nettle leaf	20111306	1
Caelo	Nettle leaf	3021401	1
Caelo	Nettle leaf	12034414	1
Caelo	Nettle leaf	13386801	1
Caelo	Nettle leaf	14344907	1
Caelo	Nettle leaf	10162712	1
Caelo	Nettle leaf	10291414	3
Caelo	Nettle leaf	12184502	2
Caelo	Nettle leaf	12184004	9
Caelo	Nettle leaf	12195002	2
Caelo	Nettle leaf	12183910	11
Caelo	Nettle leaf	10291422	3
Caelo	Nettle leaf	2381A130122	27
Caelo	Nettle leaf	72085497	1
Caelo	Nettle leaf	83374109	1
Caelo	Nettle leaf	83142389	1
Caelo	Nettle leaf	17337321	2
Caelo	Nettle leaf	12183908-3391311070	1
Caelo	Nettle leaf	12183908-3405310181	1
Caelo	Nettle leaf	12183908-3443311112	1
Caelo	Nettle leaf	12034403	8
Caelo	Nettle leaf	12034402	3
Caesar & Loretz Gm…	Nettle leaf	10291423	6
Galke	Nettle leaf	20956	1
Galke	Nettle leaf	21238	1
Galke	Nettle leaf	23302	1
Gehe	Nettle leaf	10162701	1
Gehe	Nettle leaf	2381A120619	14
Gutenberg-Apotheke	Nettle leaf	18897	1
Hepart AG	Nettle leaf	P234605kbA	1
Klenk	Nettle leaf	2381A-120619	1
Klenk	Nettle leaf	2381A150109	1
Klenk	Nettle leaf	2381A151012	1
Klenk	Nettle leaf	1107211689	1
Klenk	Nettle leaf	1913A-03054	1
Klenk	Nettle leaf	A110913	1
Klenk	Nettle leaf	2381A130703	15
Klenk	Nettle leaf	A130703	1
Klenk	Nettle leaf	2381a130703	1
Klenk	Nettle leaf	A130122	1
Klenk	Nettle leaf	2372A130703	1
Klenk	Nettle leaf	2381A140221	1
Klenk	Nettle leaf	2381A141124	1
Klenk	Nettle leaf	2381A121010	1
Klenk	Nettle leaf	114Q-03054	1
Klenk	Nettle leaf	4513E3054	1
Klenk	Nettle leaf	2381a130122	1
Klenk	Nettle leaf	2381A-121010	1
Klenk	Nettle leaf	2381A110809	1
Nachprüfung 8.2.13	Nettle leaf	C1081	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Noweda	Nettle leaf	12195001	7
Caelo	Nettle leaf	12183914	9
Sanacorp	Nettle leaf	12184707	11
Sanacorp	Nettle leaf	12184003	17
Caelo	Nettle leaf	12184005	7
Caelo	Nettle leaf	33/AD1	1
Wolf	Nettle leaf	B-821	1
Wolf	Nettle leaf	B821	1
Wolf	Nettle leaf	P234605	10
Caelo	Nettle root	10081202	1
Caelo	Nettle root	11254902	3
Caelo	Nettle root	11254903	5
Caelo	Nettle root	11265002	5
Caelo	Nettle root	11265003	2
Caelo	Nettle root	6631B130610	1
Caelo	Nettle root	11265006	1
Caelo	Nettle root	11265004	4
Caelo	Nettle root	11254904	3
Gehe	Nettle root	6631B120927	5
Caelo	Nettle root	6441A121024	1
Klenk	Nettle root	6631N110513	1
Klenk	Nettle root	6631B120416	1
Klenk	Nettle root	9931B120927	1
Sanacorp	Nettle root	11265001	2
Caelo	Nettle seed	12131505	1
Caelo	Nettle seed	13010607	1
Caelo	Nettle seed	20111301	1
Caelo	Nettle seed	13010612	2
Caelo	Nettle seed	15261608	1
Caelo	Nettle seed	17282601	1
Caelo	Nettle seed	15290602	1
Caelo	Nettle seed	16327001	3
Caelo	Nettle seed	16327003	1
Euro OTC	Nettle seed	12131507	2
Euro OTC	Nettle seed	7470A141021	2
Klenk	Nettle seed	7470A110418	1
Klenk	Nettle seed	2021505	1
Klenk	Nettle seed	7470A151009	2
Klenk	Nettle seed	7470A170130	1
Klenk	Nettle seed	7470A160928	2
Sanacorp	Nettle seed	13010602	1
Caelo	Nutmeg	12376805	1
Caelo	Nutmeg	12376802	2
Caelo	Nutmeg, powdered (spice)	12102305	2
Galke	Nutmeg, powdered (spice)	22739	1
Klenk	Nutmeg, powdered (spice)	A130304	2
Klenk	Nutmeg, powdered (spice)	7325A120903	2
Klenk	Nutmeg, powdered (spice)	7325A130304	1
Klenk	Nutmeg, powdered (spice)	7325A130515	1

O

Supplier	Substance	Batch	Spectra
Anzag 26.10.12 2.36EUR	Oak bark	10348616	6
Caelo	Oak bark	11351202	5
Bahnhof-Apotheke	Oak bark	17-121106	1
Berkel AHK	Oak bark	13360310	1
Bombastus	Oak bark	272704	1
Bombastus	Oak bark	265717	1
Bombastus	Oak bark	274392	1
Bombastus	Oak bark	274611	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Oak bark	279525	2
Bombastus	Oak bark	229090	1
Bombastus	Oak bark	286297	1
Caelo	Oak bark	15314908	2
Caelo	Oak bark	10348612	1
Caelo	Oak bark	22081204	1
Caelo	Oak bark	10348615	1
Caelo	Oak bark	7021302	1
Caelo	Oak bark	19032013	2
Caelo	Oak bark	3041301	1
Caelo	Oak bark	11351201	3
Caelo	Oak bark	11351203	1
Caelo	Oak bark	10238612	1
Caelo	Oak bark	16081305	1
Caelo	Oak bark	26081302	1
Caelo	Oak bark	5091302	1
Caelo	Oak bark	14111316	1
Caelo	Oak bark	161212	1
Caelo	Oak bark	41109-4-P	1
Caelo	Oak bark	1135121o	1
Caelo	Oak bark	123test	1
Caelo	Oak bark	13360301	1
Caelo	Oak bark	1081401	1
Caelo	Oak bark	280814A	1
Caelo	Oak bark	13360304	1
Caelo	Oak bark	13360311	1
Caelo	Oak bark	13360309	1
Caelo	Oak bark	10061504	1
Caelo	Oak bark	14277004	1
Caelo	Oak bark	14277004	2
Caelo	Oak bark	15146104	4
Caelo	Oak bark	15146103	1
Caelo	Oak bark	15146105	4
Caelo	Oak bark	15146110	1
Caelo	Oak bark	15146110	1
Caelo	Oak bark	15314904	1
Caelo	Oak bark	15314904	4
Caelo	Oak bark	15314906	1
Caelo	Oak bark	15314912	3
Caelo	Oak bark	501919	1
Caelo	Oak bark	18014702	1
Caelo	Oak bark	19133902	1
Caelo	Oak bark	18014701	1
Caelo	Oak bark	15314903	1
Caelo	Oak bark	15146109	2
Caelo	Oak bark	10348613	2
Caelo	Oak bark	11351210	8
Caelo	Oak bark	11351207-3384310110	1
Caelo	Oak bark	13360305	1
Caelo	Oak bark	13360308	1
Caelo	Oak bark	14277004	1
Caelo	Oak bark	15146105	1
Caelo	Oak bark	15314910	6
Caelo	Oak bark	13360306	2
Caelo	Oak bark	13360312	5
Caelo	Oak bark	15146101	2
Caelo	Oak bark	15146102	1
Caelo	Oak bark	10348605	1
Caelo	Oak bark	16305701	1
Caelo	Oak bark	15314901	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Oak bark	15314911	1
Caelo	Oak bark	12221102	1
Caelo	Oak bark	9357419	2
Caelo	Oak bark	12221101	9
Caelo	Oak bark	13360303	1
Caelo	Oak bark	13360306	1
Caelo	Oak bark	15314905	3
Caelo	Oak bark	12221104	2
Caelo	Oak bark	11351205	3
Caelo	Oak bark	11351208	3
Euro OTC	Oak bark		1
Galke	Oak bark	17824	2
GEHE 10.03.2014	Oak bark	761A11816	1
Gutenberg-Apotheke	Oak bark	11351206	13
Caelo	Oak bark	11351209	10
Klenk	Oak bark	C-280513-2	1
Klenk	Oak bark	761A110816	1
Klenk	Oak bark	761A090420	1
Klenk	Oak bark	761A110816	10
Noweda	Oak bark	10348617	8
Caelo	Oak bark	11351207	11
Klenk	Oak bark	761A110816	1
Caelo	Oak bark	12221105	2
Caelo	Oak bark	13360302	6
Phönix	Oak bark	10348609	2
Caelo	Oak bark, powdered	10261513	1
Caelo	Oat straw	11280008	2
Caelo	Oat straw	11280014	1
Caelo	Oat straw	11280012	2
Caelo	Oat straw	11280015	3
Caelo	Oat straw	11280017	2
Noweda	Oat straw	11280003	1
Caelo	Olive leaf	12159805	1
Caelo	Olive leaf	15254406	1
Caelo	Olive leaf	18100501	1
Klenk	Olive leaf	2211B131025	1
Klenk	Olive leaf	2211B130425	3
Klenk	Olive leaf	2211B120417	2
Klenk	Olive leaf	2211B150818	1
Klenk	Orange peel, cut	531A091125	3
Klenk	Orange peel, cut	531A130204	5
Klenk	Orange peel, cut	531a130204	1
Caelo	Oregano herb	12360904	1
Caelo	Oregano herb	11340705	1
Caelo	Oregano herb	11340708	1
Caelo	Oregano herb	11340709	1
Caelo	Oregano herb	12360901	6
Caelo	Oregano herb	11340703	2
Caelo	Oregano herb	12360902	3
Klenk	Oregano herb	4221A120315	2
Caelo	Orris root	11026704	2
Caelo	Orris root	11026706	1
Caelo	Orris root	13113401	2
Caelo	Orris root	1026706	1
Caelo	Orris root	13113404	1
Fagron	Orris root	11026705	3
Galke	Orris root	21303	1
Klenk	Orris root	B111013	1
Klenk	Orris root	6831B111013	1
Klenk	Orris root	B130102	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sanacorp	Orris root	11026701	1
Caelo	Orris root	13113402	1
Caelo	Oxycodone hydrochloride	17270202	2
Caelo	Oxycodone hydrochloride	12268912	1
Caelo	Oxycodone hydrochloride	15220205	1

P

Supplier	Substance	Batch	Spectra
Caelo	Pale coneflower root	11115206	1
Caelo	Pale coneflower root	12244504	1
Caelo	Parsley herb, rubbed	12376601	2
Caelo	Parsley herb, rubbed	51978126	1
Caelo	Parsley herb, rubbed	12376603	2
Caelo	Parsley herb, rubbed	12376602	2
Caelo	Parsley root	12080309	1
Caelo	Parsley root	12080304	1
Caelo	Parsley root	13156003	1
Caelo	Parsley root	13156005	1
Gahlke	Parsley root	20872	1
Gehe	Parsley root	6441A110210	3
Klenk	Parsley root	6441A150811	1
Klenk	Parsley root	6441A120606	5
Klenk	Parsley root	6441A121024	4
Klenk	Parsley root	6441A120283	1
Caelo	Parsley seed	PrüfNr.2814A-01550	1
Klenk	Parsley seed	7370A091120	2
Klenk	Parsley seed	7370A09120	1
an	Passionflower herb	13141212	1
Anzag	Passionflower herb	1207211669	1
Caelo	Passionflower herb	11049116	4
Caelo	Passionflower herb	12031703	2
Caelo	Passionflower herb	12031704	1
Caelo	Passionflower herb	11049108	1
Caelo	Passionflower herb	1011A-01669	1
Caelo	Passionflower herb	12031701	1
Caelo	Passionflower herb	12031715	7
Caelo	Passionflower herb	12031716	3
Caelo	Passionflower herb	12031712	1
Caelo	Passionflower herb	12101301	1
Caelo	Passionflower herb	13141201	1
Caelo	Passionflower herb	15085105	1
Caelo	Passionflower herb	12031706	3
Caelo	Passionflower herb	11049111	1
Caelo	Passionflower herb	13141202	7
Caelo	Passionflower herb	12031710	13
Caelo	Passionflower herb	12031705	4
Caelo	Passionflower herb	13141205	4
Caelo	Passionflower herb	12031714	2
Caelo	Passionflower herb	12031717	9
Caelo	Passionflower herb	13141203	2
Klenk	Passionflower herb	4231A120329	2
Klenk	Passionflower herb	A120329	2
Klenk	Passionflower herb	4231A-110913	1
Klenk	Peony root, cut	B110916	2
Klenk	Peony root, cut	6421B120327	1
Caelo	Pepper	11193911	1
Caelo	Pepper	12192304	1
Caelo	Pepper	12192306	1
Caelo	Pepper	12192305	1
Caelo	Pepper	12192309	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Pepper	15395310	1
Caelo	Pepper	13221110	1
Klenk	Pepper	A130415	2
PHOENIX 19.05.2014	Pepper	13221105	1
Bombastus	Peppermint leaf	266772	2
Bombastus	Peppermint leaf	275295	3
Bombastus	Peppermint leaf	246514	1
Bombastus	Peppermint leaf	272956	3
Bombastus	Peppermint leaf	279634	1
Bombastus	Peppermint leaf	279214	1
Bombastus	Peppermint leaf	281282	1
Bombastus	Peppermint leaf	281043	3
Bombastus	Peppermint leaf	271499	1
Bombastus	Peppermint leaf	285914	1
Bombastus	Peppermint leaf	276514	1
Bombastus	Peppermint leaf	278679	2
Bombastus	Peppermint leaf	286105	1
Bombastus	Peppermint leaf	279914	2
Bombastus	Peppermint leaf	255719	1
Bombastus	Peppermint leaf	282509	1
Caelo	Peppermint leaf	20061202	1
Caelo	Peppermint leaf	11327803	5
Caelo	Peppermint leaf	20111215	1
Caelo	Peppermint leaf	11294409	2
Caelo	Peppermint leaf	11327801	2
Caelo	Peppermint leaf	11327808	3
Caelo	Peppermint leaf	1132803	1
Caelo	Peppermint leaf	12266903	5
Caelo	Peppermint leaf	12266908	8
Caelo	Peppermint leaf	2181B090928	1
Caelo	Peppermint leaf	13030805	5
Caelo	Peppermint leaf	Int.Ch.:313011	1
Caelo	Peppermint leaf	ChB:311092	1
Caelo	Peppermint leaf	13030806	1
Caelo	Peppermint leaf	5091307	1
Caelo	Peppermint leaf	13030809	2
Caelo	Peppermint leaf	13030808	1
Caelo	Peppermint leaf	8101301	1
Caelo	Peppermint leaf	12032311	1
Caelo	Peppermint leaf	13030804	1
Caelo	Peppermint leaf	161212	1
Caelo	Peppermint leaf	12266912	1
Caelo	Peppermint leaf	13214706	1
Caelo	Peppermint leaf	6011403	1
Caelo	Peppermint leaf	13214720	1
Caelo	Peppermint leaf	14083102	2
Caelo	Peppermint leaf	14221701	1
Caelo	Peppermint leaf	14339202	2
Caelo	Peppermint leaf	13214707	3
Caelo	Peppermint leaf	268320	1
Caelo	Peppermint leaf	12054149	1
Caelo	Peppermint leaf	13030807	3
Caelo	Peppermint leaf	11294401	3
Caelo	Peppermint leaf	13214705	1
Caelo	Peppermint leaf	12266904	3
Caelo	Peppermint leaf	11347609	1
Caelo	Peppermint leaf	2181A1209-13	1
Caelo	Peppermint leaf	12032319	2
Caelo	Peppermint leaf	13105001	1
Caelo	Peppermint leaf	17117806	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Peppermint leaf	17292709	1
Caelo	Peppermint leaf	18287701	1
Caelo	Peppermint leaf	17292702	1
Caelo	Peppermint leaf	13030808-3401310161	1
Caelo	Peppermint leaf	12266908-343431160	1
Caesar & Loretz GmbH	Peppermint leaf	11294411	1
Fagron	Peppermint leaf	1234567	2
Fagron	Peppermint leaf	13030803	3
Fiebig ek:9.84EUR 24…	Peppermint leaf	2181A110512	5
Galke	Peppermint leaf	22218	1
Galke	Peppermint leaf	20975	3
Galke	Peppermint leaf	22783	3
Gehe	Peppermint leaf	2181B130717A	1
Gehe	Peppermint leaf	2181B130717B	1
Caelo	Peppermint leaf	12266913	9
Hepart AG	Peppermint leaf	B-185	5
HiperScan	Peppermint leaf		1
Klenk	Peppermint leaf	1209211505	1
Klenk	Peppermint leaf	2181A-101013	1
Klenk	Peppermint leaf	1001311505	1
Klenk	Peppermint leaf	2161A110207	1
Klenk	Peppermint leaf	1913A-01505	1
Klenk	Peppermint leaf	2161A121009	6
Klenk	Peppermint leaf	2183A120913	2
Klenk	Peppermint leaf	2161A120718	3
Klenk	Peppermint leaf	2181A130320	6
Klenk	Peppermint leaf	216A121029	1
Klenk	Peppermint leaf	2161A121206	14
Klenk	Peppermint leaf	2161	1
Klenk	Peppermint leaf	A121009	1
Klenk	Peppermint leaf	2161A111207	1
Klenk	Peppermint leaf	A130806	1
Klenk	Peppermint leaf	2181B130717	10
Klenk	Peppermint leaf	CH.2161B080818	1
Klenk	Peppermint leaf	2161A130806	7
Klenk	Peppermint leaf	2181A13020	1
Klenk	Peppermint leaf	2161B140321	1
Klenk	Peppermint leaf	2181A151119	1
Klenk	Peppermint leaf	2181a120913	3
Klenk	Peppermint leaf	2181B180727	2
Klenk	Peppermint leaf	2181A190508-06	1
Klenk	Peppermint leaf	4513E1503	1
Klenk	Peppermint leaf	2161A07020203	1
Klenk	Peppermint leaf	2181A-120913	1
Klenk	Peppermint leaf	2181A100323	1
Klenk	Peppermint leaf	2181A120913	34
Klenk	Peppermint leaf	4113Q1505	1
Klenk	Peppermint leaf	2181A171025	1
Klenk	Peppermint leaf	2181a171109	1
Klenk	Peppermint leaf	2181A190508	2
Klenk	Peppermint leaf	2161A121029	17
Klenk	Peppermint leaf	2181A180130	2
Klenk	Peppermint leaf	2161A-121206	1
Kräuter-Schulte	Peppermint leaf	56254	1
nachprüfung	Peppermint leaf	C1327	1
Noweda	Peppermint leaf	2911U-01505	1
Bombastus	Peppermint leaf	273843	2
Klenk	Peppermint leaf	2181A101013	6
Probe	Peppermint leaf	1223456	1
Wolf	Peppermint leaf	P221379	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Wolf	Peppermint leaf	B-120	1
Wolf	Peppermint leaf	B243	1
Wolf	Peppermint leaf	B-725	2
Wolf	Peppermint leaf	B725	1
	Phenobarbital	22D19-F03-384178	2
BLS	Phenobarbital	67056	5
Fagron	Phenobarbital	13G05-N09	1
Fagron	Phenobarbital	15G07-B06-311718	1
Fagron	Phenobarbital	16G20-B04-328344	3
Fagron	Phenobarbital	B01-3639508	1
Fagron	Phenobarbital	21A19-F02-376671	5
Fagron	Phenobarbital	F02-3766701	1
Fagron	Phenobarbital	19G23-B01-363958	1
Fagron	Phenobarbital	B01-3655903	1
Fagron	Phenobarbital	18C07-B01-347288	4
Fagron	Phenobarbital	19G23-B01	1
Fagron	Phenobarbital	15I18-B08-318544	1
Fagron	Phenobarbital	18H15-B01-354934	2
Fagron	Phenobarbital	19G23-B01-365593	3
Fagron	Phenobarbital	21A19-F02	3
Fagron	Phenobarbital	19G23-B01-363364	1
Fagron	Phenobarbital	B01-3549304	1
Th. Geyer	Phenobarbital	70510	17
Th. Geyer	Phenobarbital	67045	3
Caelo	Phenol	11163801	1
Caelo	Phenol	11163809	1
Caelo	Phenol	7061305	1
Caelo	Phenol	12223014	1
Caelo	Phenol	12223020	1
Caelo	Phenol	12223022	1
Caelo	Phenol	12223001	1
Caelo	Piper cubeba	11081903	1
Caelo	Podophyllum resin (from pod…	11085807	4
Caelo	Podophyllum resin (from pod…	12287805	1
Caelo	Podophyllum resin (from pod…	11085811	1
Caelo	Podophyllum resin (from pod…	12379903	1
Caelo	Podophyllum resin (from pod…	12287810	1
Caelo	Podophyllum resin (from pod…	82433349	1
Caelo	Potassium hydroxide	12057905	1
Caelo	Potassium hydroxide	11165708	1
Caelo	Potassium hydroxide	17091202	1
Caelo	Potassium hydroxide	12057912	2
Caelo	Potassium hydroxide	12057908	2
Caelo	Potassium hydroxide	12057906	1
Caelo	Potassium hydroxide	12382606	2
Caelo	Potassium hydroxide	11165705	1
Caelo	Potassium hydroxide	12382611	1
Caelo	Potassium hydroxide	27111310	1
Caelo	Potassium hydroxide	13275201	2
Caelo	Potassium hydroxide	12382601	2
Caelo	Potassium hydroxide	13275207	1
Caesar & Loretz Gm…	Potassium hydroxide	12057902	2
Caelo	Potassium hydroxide	12382603	4
Caelo	Potassium sodium tartrate t…	15375601	12
Caelo	Potassium sodium tartrate t…	17257701	4
Caelo	Potassium tartrate hemihydrate	11225007	1
Caelo	Potassium tartrate hemihydrate	27061304	1
Caelo	Potassium tartrate hemihydrate	12322110	1
Caelo	Potassium tartrate hemihydrate	13111415	1
Caelo	Potassium tartrate hemihydrate	13331113	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Potassium tartrate hemihydrate	15167703	1
Caelo	Potassium tartrate hemihydrate	24061705	1
Caelo	Potassium tartrate hemihydrate	17176002	2
Caelo	Potassium tartrate hemihydrate	19051804	1
Caelo	Potassium tartrate hemihydrate	17176004	1
Caelo	Potassium tartrate hemihydrate	17176007	1
Caelo	Potassium tartrate hemihydrate	18220301	2
Caelo	Potassium tartrate hemihydrate	193079002	1
Caelo	Potassium tartrate hemihydrate	193079004	1
Caelo	Potassium tartrate hemihydrate	18220305	2
Caelo	Potassium tartrate hemihydrate	17176001	2
Aurica / 11	Primrose flower	521301234	1
Aurica/Gehe	Primrose flower	521203308	1
Caelo	Primrose flower	11206810	5
Caelo	Primrose flower	11206808	1
Caelo	Primrose flower	5021303	1
Caelo	Primrose flower	9021301	1
Caelo	Primrose flower	11206811	1
Caelo	Primrose flower	11374403	1
Caelo	Primrose flower	25091306	1
Caelo	Primrose flower	11206807	1
Caelo	Primrose flower	1308660	1
Caelo	Primrose flower	13086608	1
Caelo	Primrose flower	13276904	1
Caelo	Primrose flower	13086603	5
Caelo	Primrose flower	11374404	1
Caelo	Primrose flower	113744044	1
Caelo	Primrose flower	11374402	1
Caelo	Primrose flower	11374401	10
Caelo	Primrose flower	13086603	1
Caelo	Primrose flower	13086602	5
Caelo	Primrose flower	10207104	1
Caelo	Primrose flower	11206803	4
Caelo	Primrose flower	11206804	1
Caelo	Primrose flower	10072509	1
Galke	Primrose flower	22612	2
Gehe	Primrose flower	11374401	1
Caelo	Primrose flower	13086605	1
Klenk	Primrose flower	1541B100414	1
Klenk	Primrose flower	B110314	1
Klenk	Primrose flower	B130808	1
Klenk	Primrose flower	A111018	1
Klenk	Primrose flower	B130808	1
Klenk	Primrose flower	1540A-100907	1
Klenk	Primrose flower	1540A100907	1
Klenk	Primrose flower	1541B110314	7
Caelo	Primrose flower	11206811	4
Caelo	Primrose flower	11374403	3
Sanacorp	Primrose flower	1541B130808	6
Caelo	Primrose flower	13086602	3
VDL	Primrose flower	11206806	1
Weltecke / GEHE	Primrose flower	63011112	1
Caelo	Primrose root, cut	13087005	3
Caelo	Primrose root, cut	10382009	1
Caelo	Primrose root, cut	10382013	1
Caelo	Primrose root, cut	12064503	1
Caelo	Primrose root, cut	10382012	1
Caelo	Primrose root, cut	12064506	4
Caelo	Primrose root, cut	24011301	1
Caelo	Primrose root, cut	5010E-02159	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Primrose root, cut	Int.Ch:318090	1
Caelo	Primrose root, cut	13087004	1
Caelo	Primrose root, cut	4021410	1
Caelo	Primrose root, cut	10382010	1
Caelo	Primrose root, cut	13067001	1
Caelo	Primrose root, cut	13087001	1
Caelo	Primrose root, cut	71653517	1
Caelo	Primrose root, cut	13087005-3534411072	1
Caelo	Primrose root, cut	13087002	4
Klenk	Primrose root, cut	6461A100511	1
Klenk	Primrose root, cut	B130218	3
Noweda	Primrose root, cut	12064504	4
Caelo	Promethazine hydrochloride	11352305	1
Caelo	Promethazine hydrochloride	19051805	1
Caelo	Promethazine hydrochloride	17058601	2
Caelo	Promethazine hydrochloride	13119211	1
Audor Pharma	Psyllium seed	15190313	2
Bahnhof-Apotheke	Psyllium seed	3-121005	1
Caelo	Psyllium seed	10291205	1
Caelo	Psyllium seed	12140301	7
Caelo	Psyllium seed	10291206	1
Caelo	Psyllium seed	12185504	10
Caelo	Psyllium seed	10291204	1
Caelo	Psyllium seed	12185509	5
Caelo	Psyllium seed	12185508	4
Caelo	Psyllium seed	12276510	1
Caelo	Psyllium seed	13305904	2
Caelo	Psyllium seed	13305903	1
Caelo	Psyllium seed	13305906	2
Caelo	Psyllium seed	13305910	4
Caelo	Psyllium seed	10061503	1
Caelo	Psyllium seed	15190304	3
Caelo	Psyllium seed	10291207	6
Caelo	Psyllium seed	13234310	3
Caelo	Psyllium seed	12185503	3
Caelo	Psyllium seed	13234309	1
Caelo	Psyllium seed	7380a120911	1
Caelo	Psyllium seed	11185811	4
Caelo	Psyllium seed	15190303	4
Caelo	Psyllium seed	11185803	1
Caelo	Psyllium seed	13305907	5
Caelo	Psyllium seed	15190306	2
Caelo	Psyllium seed	15321007	1
Caelo	Psyllium seed	12185502	1
Caesar/Noweda	Psyllium seed	11185817	3
Caesar/Noweda	Psyllium seed	12276501	3
Galke	Psyllium seed	20968	2
Galke	Psyllium seed	22989	7
Klenk	Psyllium seed	7380A150520	7
Klenk	Psyllium seed	7560a120330	1
Klenk	Psyllium seed	A120911	1
Klenk	Psyllium seed	A120109	1
Klenk	Psyllium seed	A130128	1
Klenk	Psyllium seed	7560A130418	1
Klenk	Psyllium seed	7380A150929	4
Klenk	Psyllium seed	7380A161018	2
Klenk	Psyllium seed	7380A110317	1
Klenk	Psyllium seed	7380A111018	1
Klenk	Psyllium seed	7380A130128	6
Klenk	Psyllium seed	7380A120109	24

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Psyllium seed	7380a111018	1
Klenk	Psyllium seed	7380a120109	3
Klenk	Psyllium seed	7380A120911	16
Klenk	Psyllium seed	7560A140203	1
Allianz Healthcare	Pumpkin seed	16081210	1
Caelo	Pumpkin seed	12249001	2
Caelo	Pumpkin seed	14186905	1
Caelo	Pumpkin seed	14186910	1
Caelo	Pumpkin seed	16081202	1
Caelo	Pumpkin seed	16081206	2
Caelo	Pumpkin seed	140736306	1
Caelo	Pumpkin seed	122490911	1
Caelo	Pumpkin seed	12249011	2
Caelo	Pumpkin seed	14073603	1
sanacorp	Pumpkin seed	14186909	1
Sanacorp	Pumpkin seed	16081212	1

Q

Supplier	Substance	Batch	Spectra
Caelo	Quinolinol sulfate potassiu…	7051305	1
Caelo	Quinolinol sulfate potassiu…	13071104	4
Caelo	Quinolinol sulfate potassiu…	13403501	4
Caelo	Quinolinol sulfate potassiu…	15147701	3
Caelo	Quinolinol sulfate potassiu…	15147714	1
Caelo	Quinolinol sulfate potassiu…	13403506	15
Caelo	Quinolinol sulfate potassiu…	13071101	2
Caelo	Quinolinol sulfate potassiu…	15147706	5
Caelo	Quinolinol sulfate potassiu…	10281601	1
Caelo	Quinolinol sulfate potassiu…	13071106	1
Caelo	Quinolinol sulfate potassiu…	15147708	4
Caelo	Quinolinol sulfate potassiu…	16221809	6
Caelo	Quinolinol sulfate potassiu…	13403501	3
Caelo	Quinolinol sulfate potassiu…	9106304	1
Caelo	Quinolinol sulfate potassiu…	13403513	1
Caelo	Quinolinol sulfate potassiu…	15147704	4
Caelo	Quinolinol sulfate potassiu…	16221807	6
Caelo	Quinolinol sulfate potassiu…	16221811	2
Dermapharm	Quinolinol sulfate potassiu…	100804	12
Dermapharm	Quinolinol sulfate potassiu…	140804	82
Dermapharm	Quinolinol sulfate potassiu…	120905	43
Dermapharm	Quinolinol sulfate potassiu…	1470804	1
Ebert-Jacobi	Quinolinol sulfate potassiu…	16221804	2
Lieber Leyh	Quinolinol sulfate potassiu…	1605110096	1
Nachprüfung	Quinolinol sulfate potassiu…	2812U03423	1
Nachprüfung	Quinolinol sulfate potassiu…	13071104	1
Noweda	Quinolinol sulfate potassiu…	140804	2
Phönix Gotha	Quinolinol sulfate potassiu…	120905	10

R

Supplier	Substance	Batch	Spectra
Caelo	Ramsons herb	11182207	1
Caelo	Ramsons herb	11182204	1
Caelo	Ramsons herb	11182203	1
Caelo	Ramsons herb	12380802	2
Caelo	Ramsons herb	12380801	2
Caelo	Ramsons herb	12380803	1
Caelo	Ramsons herb	14343305	1
Klenk	Ramsons herb	3511B111005	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	Ramsons herb	712914	1
-	Raspberry leaf	130849	1
AHD	Raspberry leaf	300696	1
Alfred Galke	Raspberry leaf	19851	1
an	Raspberry leaf	13086708	1
Anzag	Raspberry leaf	2291A120806	2
Anzag	Raspberry leaf	12103107	11
Anzag ek:3,00EUR 11.09.12	Raspberry leaf	12103105	18
Caelo	Raspberry leaf	1236705	1
Caelo	Raspberry leaf	10136412	1
Klenk	Raspberry leaf	2291A120507	5
Bahnhof-Apotheke	Raspberry leaf	17-120917	1
Bombastus	Raspberry leaf	274507	1
Bombastus	Raspberry leaf	279686	3
Bombastus	Raspberry leaf	273668	2
Bombastus	Raspberry leaf	269870	1
Bombastus	Raspberry leaf	291500	1
Bombastus	Raspberry leaf	273778	1
Bombastus	Raspberry leaf	272898	1
Bombastus	Raspberry leaf	248586	1
Bombastus	Raspberry leaf	267122	1
Caelo	Raspberry leaf	1310603	1
Caelo	Raspberry leaf	10013407	1
Caelo	Raspberry leaf	307211511	1
Caelo	Raspberry leaf	10013411	1
Caelo	Raspberry leaf	9081205	1
Caelo	Raspberry leaf	22081201	1
Caelo	Raspberry leaf	25091201	1
Caelo	Raspberry leaf	2909211511	1
Caelo	Raspberry leaf	9101204	1
Caelo	Raspberry leaf	18101203	1
Caelo	Raspberry leaf	12103108	8
Caelo	Raspberry leaf	11121201	1
Caelo	Raspberry leaf	12103109	2
Caelo	Raspberry leaf	17121203	1
Caelo	Raspberry leaf	1210315	1
Caelo	Raspberry leaf	12362702	7
Caelo	Raspberry leaf	8031307	1
Caelo	Raspberry leaf	10013410	1
Caelo	Raspberry leaf	18041304	1
Caelo	Raspberry leaf	12362706	29
Caelo	Raspberry leaf	11030706	3
Caelo	Raspberry leaf	21051302	1
Caelo	Raspberry leaf	IntCh:311090	1
Caelo	Raspberry leaf	11071301	1
Caelo	Raspberry leaf	20081311	1
Caelo	Raspberry leaf	12362707	5
Caelo	Raspberry leaf	13038002	1
Caelo	Raspberry leaf	13038003	1
Caelo	Raspberry leaf	13101803	1
Caelo	Raspberry leaf	12362711	9
Caelo	Raspberry leaf	12362708	4
Caelo	Raspberry leaf	10136408	1
Caelo	Raspberry leaf	7011402	1
Caelo	Raspberry leaf	9011404	1
Caelo	Raspberry leaf	13127901	3
Caelo	Raspberry leaf	30011408	1
Caelo	Raspberry leaf	14018803	1
Caelo	Raspberry leaf	12103101	7

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Raspberry leaf	2271C120508	5
Caelo	Raspberry leaf	12362704	5
Caelo	Raspberry leaf	713E-01511	1
Caelo	Raspberry leaf	11030707	4
Caelo	Raspberry leaf	12362705	9
Caelo	Raspberry leaf	314U1511	1
Caelo	Raspberry leaf	12392709	1
Caelo	Raspberry leaf	6859427	1
Caelo	Raspberry leaf	12368706	1
Caelo	Raspberry leaf	12362709	7
Caelo	Raspberry leaf	231013c	1
Caelo	Raspberry leaf	10136404	1
Caelo	Raspberry leaf	12362710	14
Caelo	Raspberry leaf	12362710-3432311160	1
Caelo	Raspberry leaf	13101604	3
Caelo	Raspberry leaf	13101602-347312141	1
Caesar & Loretz Gm...	Raspberry leaf	10013408	1
China Medica	Raspberry leaf	13086703	1
Galke	Raspberry leaf	21244	1
Galke	Raspberry leaf	18060	2
Galke	Raspberry leaf	19499	2
Galke	Raspberry leaf	23532	1
gehe 10.12.13	Raspberry leaf	229117121120	1
Gutenberg-Apotheke	Raspberry leaf	28911	1
Klenk	Raspberry leaf	2291A12112o	1
Caelo	Raspberry leaf	11030705	1
Caelo	Raspberry leaf	13101605	1
Kenk / Phoenix	Raspberry leaf	22781C120508	1
Klenk	Raspberry leaf	2291A-120806	1
Klenk	Raspberry leaf	12273107	1
Klenk	Raspberry leaf	2291A130320	1
Klenk	Raspberry leaf	A130430	1
Klenk	Raspberry leaf	2291A121120	4
Klenk	Raspberry leaf	2291A120813	2
Klenk	Raspberry leaf	2291a111124	1
Klenk	Raspberry leaf	2291A110125	1
Phoenix	Raspberry leaf	10136409	1
Caelo	Raspberry leaf	12130107	1
Phönix	Raspberry leaf	12362701	7
Caelo	Raspberry leaf	12103111	15
Klenk	Raspberry leaf	2291A111124	1
Sanacorp	Raspberry leaf	12362703	9
Sanacorp	Raspberry leaf	13038001	6
Caelo	Raspberry leaf	10013409	2
Caelo	Raspberry leaf	13101603	6
Caelo	Raspberry leaf	11030704	2
VDL	Raspberry leaf	10013406	3
Wolf	Raspberry leaf	P201727	19
Wolf	Raspberry leaf	P222676	1
Wolf	Raspberry leaf	B-457	1
Aurica	Red clover flower	521206331	1
Aurica	Red clover flower	521203442	1
Aurica/Anzag	Red clover flower	521303918	1
Galke	Red clover flower	23128	2
Klenk	Red clover flower	7470A130311	1
Klenk	Red clover flower	811Q-07163	1
Klenk	Red clover flower	1640A110727	1
Klenk	Red clover flower	1640a130122	1
Klenk	Red clover flower	1640A130122	15
Kräuter Schulte	Red clover flower	53778	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Red poppy petals, cut	12330205	1
Kräuter Schulte	Red tea	52029	1
Caelo	Red-rose Flower	12380008	2
Galke	Red-rose Flower	22641	2
Klenk	Red-rose Flower	1561A121016	1
Caelo	Red-rose Flower	12380004	1
Klenk	Red-rose petal	1561A110404	1
Caelo	Red-rose petal	10306514	1
Caelo	Red-rose petal	11304901	3
Caelo	Red-rose petal	11304906	1
Caelo	Red-rose petal	11304904	4
Caelo	Red-rose petal	11011301	1
Caelo	Red-rose petal	12380001	4
Caelo	Red-rose petal	11304912	2
Caelo	Red-rose petal	12380008	1
Caelo	Red-rose petal	13194403	4
Caelo	Red-rose petal	10113211	1
Caelo	Red-rose petal	12380007-3357319071	1
Caelo	Red-rose petal	12380004	2
Caelo	Red-rose petal	13194402	1
Klenk	Red-rose petal	1561B101210	2
Klenk	Red-rose petal	1561A121016-34023101	1
kräuter schulte	Red-rose petal	47543	1
Richter	Red-rose petal	P236157	1
Caelo	Redwood, cut	12049608	2
Caelo	Redwood, cut	12041403	1
Caelo	Redwood, cut	13106901	1
Caelo	Redwood, cut	12049607	2
Klenk	Redwood, cut	5961B111219	1
Caelo	Restharrow root	71035467	1
Bombastus	Restharrow root	274421	1
Bombastus	Restharrow root	272831	2
Bombastus	Restharrow root	283708	1
Caelo	Restharrow root	11247302	2
Caelo	Restharrow root	11103105	2
Caelo	Restharrow root	6101201	1
Caelo	Restharrow root	20111213	1
Caelo	Restharrow root	21011306	1
Caelo	Restharrow root	12330001	14
Caelo	Restharrow root	1233001	2
Caelo	Restharrow root	Int.Ch:212150	1
Caelo	Restharrow root	12330005	5
Caelo	Restharrow root	15101313	1
Caelo	Restharrow root	4021406	1
Caelo	Restharrow root	12330002	1
Caelo	Restharrow root	12330003	2
Caelo	Restharrow root	1230004	1
Caelo	Restharrow root	72439069	1
Caesar/Noweda	Restharrow root	71015/3	2
Galke	Restharrow root	12700	1
Hepart AG	Restharrow root	B130404	3
Klenk	Restharrow root	6411111110	1
Klenk	Restharrow root	6411B101216	2
Klenk	Restharrow root	4296345	1
Klenk	Restharrow root	6411B111110	1
Klenk	Restharrow root	B111110	1
Klenk	Restharrow root	6411B130404	2
Caelo	Restharrow root	11103107	2
Caelo	Rhubarb	11265902	1
Caelo	Rhubarb	11057810	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Rhubarb	12211903	4
Caelo	Rhubarb	11057818	2
Caelo	Rhubarb	10071302	1
Caelo	Rhubarb	12211908	1
Caelo	Rhubarb	11321806	1
Caelo	Rhubarb	15101301	1
Caelo	Rhubarb	13235201	2
Caelo	Rhubarb	25111305	1
Caelo	Rhubarb	14155404	1
Caelo	Rhubarb	12211904	2
Caelo	Rhubarb	12211902	3
Caelo	Rhubarb	13235205	1
Caelo	Rhubarb	11057804	1
Caelo	Rhubarb	12211906	1
Caelo	Rhubarb	13235203	1
Gehe	Rhubarb	13235208	2
Klenk	Rhubarb	6891B111118	1
Klenk	Rhubarb	7761B130514	2
Phoenix	Rhubarb	11057817	3
Phönix	Rhubarb	12211905	3
vedono	Rhubarb	12211907	6
Bombastus	Rhubarb, powdered	11043806	1
Caelo	Rhubarb, powdered	11043819	2
Caelo	Rhubarb, powdered	9071201	1
Caelo	Rhubarb, powdered	11043817	1
Caelo	Rhubarb, powdered	11043818	1
Caelo	Rhubarb, powdered	11043816	1
Caelo	Rhubarb, powdered	11043826	1
Caelo	Rhubarb, powdered	13193106	2
Caelo	Rhubarb, powdered	23061402	1
Caelo	Rhubarb, powdered	11043809	1
Caelo	Rhubarb, powdered	11043816	2
Caelo	Rhubarb, powdered	11043818	1
Caelo	Rhubarb, powdered	11043825	2
Caelo	Rhubarb, powdered	11043822	1
Caelo	Rhubarb, powdered	13193104	4
Caelo	Rhubarb, powdered	13193109	1
Fagron	Rhubarb, powdered	11043821	1
Hedinger	Rhubarb, powdered	13193110	1
Caelo	Ribwort plantain	13113007	6
Bahnhof-Apotheke	Ribwort plantain	7-121011	1
Bombastus	Ribwort plantain	276453	1
Bombastus	Ribwort plantain	275479	1
Caelo	Ribwort plantain	13113008	5
Caelo	Ribwort plantain	23121304	1
Caelo	Ribwort plantain	10315707	2
Caelo	Ribwort plantain	8061208	1
Caelo	Ribwort plantain	17071201	1
Caelo	Ribwort plantain	10315715	9
Caelo	Ribwort plantain	10315712	2
Caelo	Ribwort plantain	15101204	1
Caelo	Ribwort plantain	10315711	4
Caelo	Ribwort plantain	20111208	1
Caelo	Ribwort plantain	12225802	5
Caelo	Ribwort plantain	19121202	1
Caelo	Ribwort plantain	12225804	1
Caelo	Ribwort plantain	12362902	7
Caelo	Ribwort plantain	22021302	1
Caelo	Ribwort plantain	2031302	1
Caelo	Ribwort plantain	12362906	7

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Ribwort plantain	25041301	1
Caelo	Ribwort plantain	13113001	8
Caelo	Ribwort plantain	11061304	1
Caelo	Ribwort plantain	28061301	1
Caelo	Ribwort plantain	25091305	1
Caelo	Ribwort plantain	1362903	1
Caelo	Ribwort plantain	16101304	1
Caelo	Ribwort plantain	13113005	5
Caelo	Ribwort plantain	15111302	1
Caelo	Ribwort plantain	20111304	1
Caelo	Ribwort plantain	10011402	1
Caelo	Ribwort plantain	13113010	4
Caelo	Ribwort plantain	4021411	1
Caelo	Ribwort plantain	13410603	3
Caelo	Ribwort plantain	13410601	1
Caelo	Ribwort plantain	13410612	1
Caelo	Ribwort plantain	14199202	1
Caelo	Ribwort plantain	15096301	1
Caelo	Ribwort plantain	15096308	1
Caelo	Ribwort plantain	13232401	1
Caelo	Ribwort plantain	10315705	1
Caelo	Ribwort plantain	1313007	1
Caelo	Ribwort plantain	10315714	2
Caelo	Ribwort plantain	10328702	2
Caelo	Ribwort plantain	12225803	2
Caelo	Ribwort plantain	12362903-3388311070	1
Caelo	Ribwort plantain	13113004-3488312172	1
Caelo	Ribwort plantain	13113006	6
Caesar & Loretz Gm…	Ribwort plantain	12362903	33
Caesar & Loretz Gm…	Ribwort plantain	13113004	13
Cealo	Ribwort plantain	12362907	2
Galke	Ribwort plantain	20259	1
Galke	Ribwort plantain	21598	1
Gehe	Ribwort plantain	1080413	1
Hepart AG	Ribwort plantain	20832	5
Klenk	Ribwort plantain	4271A130115	6
Klenk	Ribwort plantain	4271A-110816	1
Klenk	Ribwort plantain	A110816	1
Klenk	Ribwort plantain	4271A130716	1
Klenk	Ribwort plantain	4281N111121	1
Klenk	Ribwort plantain	4271A111125	2
Klenk	Ribwort plantain	4271A100615	2
Klenk	Ribwort plantain	4271A110816	2
Klenk	Ribwort plantain	427A111125	1
Phoenix	Ribwort plantain	4271A11016	1
Sanacorp	Ribwort plantain	263401	1
Caelo	Ribwort plantain	12362901	1
C	Robert herb	11147810	3
Caelo	Robert herb	11147807	3
Caelo	Robert herb	11147804	1
Caelo	Robert herb	8121203	1
Caelo	Robert herb	11147813	2
Caelo	Robert herb	12319305	1
Caelo	Robert herb	12319304	2
Caelo	Robert herb	11147812	3
Caelo	Robert herb	12319302	1
Klenk	Robert herb	A110621	6
Klenk	Robert herb	3951A110621	7
Klenk	Robert herb	3951B121218	2
Klenk	Robert herb	3951B12118	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Rose hips peel	12064207	1
Bombastus	Rose hips peel	275394	2
Bombastus	Rose hips peel	283458	1
Bombastus	Rose hips peel	257166	1
Bombastus	Rose hips peel	277431	3
Bombastus	Rose hips peel	285184	1
Bombastus	Rose hips peel	231013A	1
Caelo	Rose hips peel	15061210	1
Caelo	Rose hips peel	25061203	1
Caelo	Rose hips peel	11301405	2
Caelo	Rose hips peel	10101206	1
Caelo	Rose hips peel	11301401	1
Caelo	Rose hips peel	7031305	1
Caelo	Rose hips peel	12288301	1
Caelo	Rose hips peel	12357501	1
Caelo	Rose hips peel	12357505	6
Caelo	Rose hips peel	5091301	1
Caelo	Rose hips peel	12357504	2
Caelo	Rose hips peel	9121301	1
Caelo	Rose hips peel	14050704	1
Caelo	Rose hips peel	14050705	1
Caelo	Rose hips peel	2851A120904konv.	1
Caelo	Rose hips peel	10157309	1
Caelo	Rose hips peel	13317805	1
Caelo	Rose hips peel	11301403	2
Caelo	Rose hips peel	13317801	2
Caelo	Rose hips peel	12357502	3
Klenk	Rose hips peel	2851A150310	4
Klenk	Rose hips peel	2851A101119	3
Klenk	Rose hips peel	2851A110202	1
Klenk	Rose hips peel	2841B111019	2
Klenk	Rose hips peel	2851A120102	5
Klenk	Rose hips peel	2851A120904	2
Klenk	Rose hips peel	A120904	3
Klenk	Rose hips peel	2851A-110202	1
Klenk	Rose hips peel	3613M-01543	1
Caelo	Rose hips peel	11301407	12
Caelo	Rose hips peel	12288302	7
Aurica	Rose hips with peel, cut	521201801	1
Caelo	Rose hips with peel, cut	307211542	1
Caelo	Rose hips with peel, cut	16111201	1
Caelo	Rose hips with peel, cut	19111204	1
Caelo	Rose hips with peel, cut	12064207	2
Caelo	Rose hips with peel, cut	1512211542	1
Caelo	Rose hips with peel, cut	12064210	3
Caelo	Rose hips with peel, cut	2103311542	1
Caelo	Rose hips with peel, cut	12064209	4
Caelo	Rose hips with peel, cut	12029011	1
Caelo	Rose hips with peel, cut	12064213	1
Caelo	Rose hips with peel, cut	13048703	1
Caelo	Rose hips with peel, cut	13048704	1
Caelo	Rose hips with peel, cut	13048704	3
Caelo	Rose hips with peel, cut	12029008	1
Caelo	Rose hips with peel, cut	12064210	2
Caelo	Rose hips with peel, cut	12064212	3
Caelo	Rose hips with peel, cut	12064201	1
Caelo	Rose hips with peel, cut	12064209	1
Caelo	Rose hips with peel, cut	12064213	1
Caelo	Rose hips with peel, cut	13048703	1
Caelo	Rose hips with peel, cut	12064202	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Rose hips with peel, cut	12064207	3
Caelo	Rose hips with peel, cut	13048701	2
Caelo	Rose hips with peel, cut	114Q-01542	1
Caelo	Rose hips with peel, cut	13097405	1
Caelo	Rose hips with peel, cut	12064212	2
Klenk	Rose hips with peel, cut	B111019	1
Klenk	Rose hips with peel, cut	A120719	1
Klenk	Rose hips with peel, cut	B130523	1
Klenk	Rose hips with peel, cut	A120904	1
Klenk	Rose hips with peel, cut	2841B081210	1
Klenk	Rose hips with peel, cut	2841B111019	3
Klenk	Rose hips with peel, cut	3613M-01542	1
Klenk	Rose hips with peel, cut	2851A120904	1
Phönix	Rose hips with peel, cut	10281021	1
Phönix	Rose hips with peel, cut	2841B130523	1
Phönix	Rose hips with peel, cut	2841B130523	1
Caelo	Rose hips with peel, cut	12064202	1
Caelo	Rose hips with peel, cut	12064206	1
Caelo	Rose mallow flower, cut	13040402	1
Caelo	Rose mallow flower, cut	13040401	2
Caelo	Rose mallow flower, cut	10244507	1
an	Roselle	14018101	1
Caelo	Roselle	12267502	4
Caelo	Roselle	11036504	1
Caelo	Roselle	11036512	1
Caelo	Roselle	7121301	1
Caelo	Roselle	12267507	2
Caelo	Roselle	12267504	3
Caelo	Roselle	12007306	1
Caelo	Roselle	11036509	2
Caelo	Roselle	12267503	2
Caelo	Roselle	12267501	3
Caelo	Roselle	12267502	3
Caelo	Roselle	12267504	1
Caelo	Roselle	12267504-3428311150	1
Caelo	Roselle	11036511	1
Klenk	Roselle	1431B130205	1
Klenk	Roselle	B130205	1
Klenk	Roselle	1431B-110519	1
Klenk	Roselle	1431B131015	2
Klenk	Roselle	1431B111122	1
Sanacorp	Roselle	12267508	2
vedono	Roselle	12007313	1
Akazie	Rosemary leaf	20.09.2015	1
Bahnhof-Apotheke	Rosemary leaf	7-120915	1
Bomastus-Werke/Phönix	Rosemary leaf	298424	2
Bombastus	Rosemary leaf	277128	1
Bombastus	Rosemary leaf	293920	1
Bombastus	Rosemary leaf	281248	1
Bombastus	Rosemary leaf	287805	1
Bombastus	Rosemary leaf	270171	1
Bombastus	Rosemary leaf	281843	1
Caelo	Rosemary leaf	11193402	2
Caelo	Rosemary leaf	11193405	1
Caelo	Rosemary leaf	11193404	1
Caelo	Rosemary leaf	11193408	6
Caelo	Rosemary leaf	5041302	1
Caelo	Rosemary leaf	IntCh:313060	1
Caelo	Rosemary leaf	12225902	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Rosemary leaf	13128801	1
Caelo	Rosemary leaf	13128802	2
Caelo	Rosemary leaf	13128806	2
Caelo	Rosemary leaf	13128805	1
Caelo	Rosemary leaf	28051404	1
Caelo	Rosemary leaf	14082901	1
Caelo	Rosemary leaf	14159601	1
Caelo	Rosemary leaf	1415901	1
Caelo	Rosemary leaf	2261A7020901	1
Caelo	Rosemary leaf	17352502	1
Caelo	Rosemary leaf	11193406	1
Caelo	Rosemary leaf	11193405	1
Caelo	Rosemary leaf	15125001	2
Caelo	Rosemary leaf	15125008	1
Caelo	Rosemary leaf	15428003	1
Galke	Rosemary leaf	21390	1
Galke	Rosemary leaf	19813	1
Galke	Rosemary leaf	22777	1
Klenk	Rosemary leaf	301401	1
Klenk	Rosemary leaf	2261A120224	18
Klenk	Rosemary leaf	A130201	2
Klenk	Rosemary leaf		1
Klenk	Rosemary leaf	61A131118	1
Klenk	Rosemary leaf	2261A170803	1
Klenk	Rosemary leaf	2261A140910	4
Klenk	Rosemary leaf	2216A170803	1
Klenk	Rosemary leaf	2261A130201	29
Klenk	Rosemary leaf	2261A160329	2
Klenk	Rosemary leaf	112E-01510	1
Klenk	Rosemary leaf	2261A160905	6
Klenk	Rosemary leaf	2261A150622	6
Klenk	Rosemary leaf	2261A081117	1
Klenk	Rosemary leaf	2261a160329	1
Klenk	Rosemary leaf	2261A131118	13
Noweda	Rosemary leaf	2261A100916	1
Noweda	Rosemary leaf	15428011	1
Klenk	Rosemary leaf	2261a120224	2
Klenk	Rosemary leaf	2261A170317	1
Caelo	Rue herb, cut		1
Caelo	Rue herb, cut	9336802	1
Caelo	Rue herb, cut	12148804	1
Caelo	Rue herb, cut	12148806	1
Caelo	Rue herb, cut	12148801	1
Caelo	Rue herb, cut	11371803	1
Caelo	Rue herb, cut	12148803	2
Gehe	Rue herb, cut	12148802	1
Klenk	Rue herb, cut	A120207	1
Klenk	Rue herb, cut	4361A120207	1
Klenk	Rue herb, cut	4361A07020601	1
Klenk	Rue herb, cut	4361A100707	3
Fagron	Rutoside trihydrate	13K12-B06	1
Fagron	Rutoside trihydrate	13K12-B06295483	1
Fagron	Rutoside trihydrate	13K12B06295483	1
Fagron	Rutoside trihydrate	L14050127	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra

S

Supplier	Substance	Batch	Spectra
Klenk	Saffron	384A110608	1
Klenk	Saffron	384A-120410	1
Klenk	Saffron	384A130320	2
Klenk	Saffron	384a120410	1
Caelo	Saffron filaments	10184811	2
Caelo	Saffron filaments	11071310	1
Caelo	Saffron filaments	15101305	1
Caelo	Saffron filaments	21011403	1
Caelo	Saffron filaments	12108311	2
Caelo	Saffron filaments	10184822	1
Caelo	Saffron filaments	12108308	2
Fagron	Saffron filaments	380A120416	1
Klenk	Saffron filaments	380A130613	1
Anzag ek: 3,06 11....	Sage leaf	2301A120403	38
Aurica	Sage leaf	521204613	1
Bahnhof-Apotheke	Sage leaf	3-121018	1
Bombastus	Sage leaf	270115	1
Bombastus	Sage leaf	271253	1
Bombastus	Sage leaf	277512	1
Bombastus	Sage leaf	255381	1
Caelo	Sage leaf	11056109	5
Caelo	Sage leaf	22061201	1
Caelo	Sage leaf	22081203	1
Caelo	Sage leaf	31081202	1
Caelo	Sage leaf	1209211513	1
Caelo	Sage leaf	11056123	5
Caelo	Sage leaf	410211513	1
Caelo	Sage leaf	111012004	1
Caelo	Sage leaf	11056125	3
Caelo	Sage leaf	11347508	3
Caelo	Sage leaf	12112101	1
Caelo	Sage leaf	22111203	1
Caelo	Sage leaf	15121201	1
Caelo	Sage leaf	20121201	1
Caelo	Sage leaf	11347511	9
Caelo	Sage leaf	11347509	4
Caelo	Sage leaf	12021302	1
Caelo	Sage leaf	103311513	1
Caelo	Sage leaf	12370001	18
Caelo	Sage leaf	15041304	1
Caelo	Sage leaf	11347513	1
Caelo	Sage leaf	12370006	8
Caelo	Sage leaf	17061302	1
Caelo	Sage leaf	25061302	1
Caelo	Sage leaf	312010	1
Caelo	Sage leaf	26081301	1
Caelo	Sage leaf	12370004	2
Caelo	Sage leaf	14111315	1
Caelo	Sage leaf	9121302	1
Caelo	Sage leaf	12370015	2
Caelo	Sage leaf	8011420	1
Caelo	Sage leaf	13011405	1
Caelo	Sage leaf	12370017	1
Caelo	Sage leaf	13266603	2
Caelo	Sage leaf	13266605	3
Caelo	Sage leaf	13266606	1
Caelo	Sage leaf	13266621	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sage leaf	13266626	1
Caelo	Sage leaf	12370013	3
Caelo	Sage leaf	279939	1
Caelo	Sage leaf	11347503	1
Caelo	Sage leaf	12380009	1
Caelo	Sage leaf	1237003	1
Caelo	Sage leaf	123770010	1
Caelo	Sage leaf	12370011	11
Caelo	Sage leaf	12370003-3359319071	1
Caelo	Sage leaf	12370014-3477312161	1
Caelo	Sage leaf	12370014	8
Caelo	Sage leaf	12370009	12
Caesar & Loretz Gm...	Sage leaf	11056121	3
Caesar & Loretz Gm...	Sage leaf	11347502	5
Caesar & Loretz Gm...	Sage leaf	12370002	4
Caesar & Loretz Gm...	Sage leaf	12370010	16
Caesar & Loretz Gm...	Sage leaf	12370016	9
Finze	Sage leaf	2301A110204	7
Galke	Sage leaf	21015	3
gehe 07.12.2013	Sage leaf	2301/7120403	1
Kenk / Phoenix	Sage leaf	2301A130904	2
Klenk	Sage leaf	C120126	1
Klenk	Sage leaf	2301A110420	1
Klenk	Sage leaf	2301C12126	1
Klenk	Sage leaf	2301a120403	1
Klenk	Sage leaf	2301c120126	1
Klenk	Sage leaf	2301C12026	1
Klenk	Sage leaf	2301C120126	16
Klenk	Sage leaf	2301A110420	2
Nachprüfung 21.11.11	Sage leaf	C1247	1
Phoenix	Sage leaf	231C130326	1
Caelo	Sage leaf	12370003	4
Wolf	Sage leaf	B735	1
Galke	Sanicle herb, cut	23097	1
Kräuter Schulte	Saponaria root, cut	54524	2
Kräuter Schulte	Saponaria root, cut	54977	1
Kräuter Schulte	Saponaria root, cut	54500	1
Caelo	Sarsaparilla root, cut	13079201	1
Klenk	Sarsaparilla root, cut	6561B111108	1
Klenk	Sarsaparilla root, cut	B111108	1
bohn	Savory, rubbed	12177208	1
Caelo	Savory, rubbed	12177203	7
Caelo	Savory, rubbed	12200801	1
Caelo	Savory, rubbed	12177201	1
Caelo	Savory, rubbed	12177207	2
Caelo	Savory, rubbed	13172404	2
Hepart AG	Savory, rubbed	12177205	3
Bomba/AHD	Senna leaflet	280008	1
Bombastus	Senna leaflet	280448	1
Bombastus	Senna leaflet	273547	3
Bombastus	Senna leaflet	278109	1
Bombastus	Senna leaflet	273474	1
Bombastus	Senna leaflet	280581	2
Caelo	Senna leaflet	11277304	4
Caelo	Senna leaflet	806211514	1
Caelo	Senna leaflet	11277305	1
Caelo	Senna leaflet	11277316	4
Caelo	Senna leaflet	18071201	1
Caelo	Senna leaflet	2909211514	1
Caelo	Senna leaflet	711211514	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Senna leaflet	1273103	1
Caelo	Senna leaflet	12273107	9
Caelo	Senna leaflet	103311514	2
Caelo	Senna leaflet	12273105	6
Caelo	Senna leaflet	1803311514	1
Caelo	Senna leaflet	11041009	1
Caelo	Senna leaflet	12273114	2
Caelo	Senna leaflet	2231B13014	1
Caelo	Senna leaflet	2413Q01514	1
Caelo	Senna leaflet	12273120	5
Caelo	Senna leaflet	12115502	1
Caelo	Senna leaflet	9071302	1
Caelo	Senna leaflet	12276111	1
Caelo	Senna leaflet	313082	1
Caelo	Senna leaflet	5091306	1
Caelo	Senna leaflet	13136703	3
Caelo	Senna leaflet	1316703	2
Caelo	Senna leaflet	15101303	1
Caelo	Senna leaflet	111113a	1
Caelo	Senna leaflet	21011401	1
Caelo	Senna leaflet	12369903	1
Caelo	Senna leaflet	14183805	2
Caelo	Senna leaflet	14306310	1
Caelo	Senna leaflet	14306311	2
Caelo	Senna leaflet	14306324	1
Caelo	Senna leaflet	12273106	3
Caelo	Senna leaflet	12273115	11
Caelo	Senna leaflet	10126502	1
Caelo	Senna leaflet	12273111	10
Caelo	Senna leaflet	19135513	3
Caelo	Senna leaflet	19135519	2
Caelo	Senna leaflet	191355003	1
Caelo	Senna leaflet	12273118	3
Caelo	Senna leaflet	3813E1514	1
Caelo	Senna leaflet	4113Q1514	1
Caelo	Senna leaflet	5013U01514	1
Caelo	Senna leaflet	131316701	1
Caelo	Senna leaflet	2331B120521	4
Caelo	Senna leaflet	514R1514	1
Caelo	Senna leaflet	18046104	2
Caelo	Senna leaflet	18046209	1
Caelo	Senna leaflet	12273104	2
Caelo	Senna leaflet	18046110	1
Caelo	Senna leaflet	19135501	1
Caelo	Senna leaflet	12115503	6
Caelo	Senna leaflet	12273113	3
Caelo	Senna leaflet	12273119	4
Caelo	Senna leaflet	13136704	13
Caelo	Senna leaflet	13136705-3489312103	1
Caelo	Senna leaflet	13136706	1
Caelo	Senna leaflet	1316706	1
Caesar & Loretz Gm…	Senna leaflet	11277303	3
Caesar & Loretz Gm…	Senna leaflet	11277308	3
Caesar & Loretz Gm…	Senna leaflet	11277314	5
Caesar & Loretz Gm…	Senna leaflet	12273103	11
Caesar & Loretz Gm…	Senna leaflet	13136708	7
Caesar&Loretz GmbH…	Senna leaflet	12115504	4
Cealo	Senna leaflet	12273116	15
Fagron	Senna leaflet	314Q1514	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Galke	Senna leaflet	21778	1
Caelo	Senna leaflet	13136705	4
Klenk	Senna leaflet	2331A100525	2
Klenk	Senna leaflet	2331B120403	1
Klenk	Senna leaflet	2331B150903	1
Klenk	Senna leaflet	2331B110907	2
Klenk	Senna leaflet	2331C120614	8
Klenk	Senna leaflet	2331B130214	5
Klenk	Senna leaflet	B130214	1
Klenk	Senna leaflet	2331C130326	16
Klenk	Senna leaflet	2331c130326	1
Klenk	Senna leaflet	2331A110207	1
Caelo	Senna leaflet	13136718	1
Caelo	Senna leaflet	13136724	1
Phönix 10.01.2014	Senna leaflet	13136707	1
Sanacorp	Senna leaflet	13136701	6
Caelo	Senna leaflet	11277307	1
Caelo	Senna leaflet	11277301	1
Caelo	Senna leaflet	12115501	5
Caelo	Senna leaflet	12273101	4
Caelo	Senna leaflet, powdered	11193307	1
Caelo	Senna leaflet, powdered	15363922	1
Caelo	Senna leaflet, powdered	17223202	1
Caelo	Senna leaflet, powdered	14347606	1
Caleo/ Fiebig	Senna leaflet, powdered	15363902	1
Fiebig	Senna leaflet, powdered	15363920	1
Klenk	Senna leaflet, powdered	2331B150903	1
Caelo	Senna pods, tinnevelly	11003004	1
Caelo	Senna pods, tinnevelly	11003009	2
Caelo	Senna pods, tinnevelly	22061202	1
Caelo	Senna pods, tinnevelly	110030009	1
Caelo	Senna pods, tinnevelly	12267604	1
Caelo	Senna pods, tinnevelly	12267609	3
Caelo	Senna pods, tinnevelly	11003013	1
Caelo	Senna pods, tinnevelly	122676707	1
Caelo	Senna pods, tinnevelly	12267606	1
Caelo	Senna pods, tinnevelly	12267602	2
Caelo	Senna pods, tinnevelly	12267610	1
Caelo	Senna pods, tinnevelly	12267608	1
Caelo	Senna pods, tinnevelly	12267007	1
Caelo	Senna pods, tinnevelly	12267201	1
Caelo	Senna pods, tinnevelly	17030712	1
Caelo	Senna pods, tinnevelly	18240501	1
Caelo	Senna pods, tinnevelly	18240505	1
Caelo	Senna pods, tinnevelly	17030709	1
Caelo	Senna pods, tinnevelly	17030708	1
Caelo	Senna pods, tinnevelly	18240506	1
Caelo	Senna pods, tinnevelly	12267605	1
Caesar & Loretz Gm...	Senna pods, tinnevelly	11003012	1
Caesar & Loretz Gm...	Senna pods, tinnevelly	11003014	1
Caesar & Loretz Gm...	Senna pods, tinnevelly	12267601	2
Caesar & Loretz Gm...	Senna pods, tinnevelly	12267603	1
Klenk	Senna pods, tinnevelly	1041B120327	2
Alfred Galke	Shepherd's purse	20591	1
Bahnhof-Apotheke	Shepherd's purse	4-120924	1
Bombastus	Shepherd's purse	269594	4
Bombastus	Shepherd's purse	278856	2
Bombastus	Shepherd's purse	269977	1
Bombastus	Shepherd's purse	284136	1
Bombastus	Shepherd's purse	12345	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Shepherd's purse	287350	1
Caelo	Shepherd's purse	11036406	5
Caelo	Shepherd's purse	14061201	1
Caelo	Shepherd's purse	11091202	1
Caelo	Shepherd's purse	15101202	1
Caelo	Shepherd's purse	1132820111-14	1
Caelo	Shepherd's purse	11328203	5
Caelo	Shepherd's purse	11328204	3
Caelo	Shepherd's purse	269595	1
Caelo	Shepherd's purse	12354201	11
Caelo	Shepherd's purse	11328209	6
Caelo	Shepherd's purse	11328205	1
Caelo	Shepherd's purse	10061301	1
Caelo	Shepherd's purse	12354202	2
Caelo	Shepherd's purse	12354204	16
Caelo	Shepherd's purse	12354203	13
Caelo	Shepherd's purse	12354001	1
Caelo	Shepherd's purse	3121301	1
Caelo	Shepherd's purse	12354207	2
Caelo	Shepherd's purse	12354209	1
Caelo	Shepherd's purse	12354206	5
Caelo	Shepherd's purse	11036401	1
Caelo	Shepherd's purse	12354503	1
Caelo	Shepherd's purse	11328201	6
Caelo	Shepherd's purse	11328208	6
Caelo	Shepherd's purse	12354203-3396310111	1
Caelo	Shepherd's purse	11328207	8
Caelo	Shepherd's purse	11328206	2
Caelo	Shepherd's purse	12254202	1
Caelo	Shepherd's purse	12354205	6
Caelo	Shepherd's purse	11036404	1
Galke	Shepherd's purse	21719	2
Galke	Shepherd's purse	19483	1
Klenk	Shepherd's purse	3671A-100414	2
Klenk	Shepherd's purse	3671B111201	1
Klenk	Shepherd's purse	B111201	1
Caelo	Shepherd's purse	13344203	1
Caelo	Shepherd's purse	11036410	2
Wolf	Shepherd's purse	B449	2
-	Silverweed	711M-01619	1
-	Silverweed	130849	1
Caelo	Silverweed	20081202	1
Caelo	Silverweed	8111204	1
Caelo	Silverweed	11016407	1
Caelo	Silverweed	11328109	13
Caelo	Silverweed	11328110	1
Caelo	Silverweed	11328105	7
Caelo	Silverweed	11328112	2
Caelo	Silverweed	11016404	1
Galke	Silverweed	12891	2
Gehe	Silverweed	11328101	1
Klenk	Silverweed	3551A110913	1
Klenk	Silverweed	H-280513-3	1
Klenk	Silverweed	A110913	2
Klenk	Silverweed	3551A130903	1
Phönix	Silverweed	11328107	7
Klenk	Silverweed	11328103	4
Euro OTC	Sodium alginate	1509036-01	1
Fagron	Sodium alginate	14G22-B99	1
phönix	Sodium alginate	11509036-02	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Sigma-Aldrich	Sodium butyrate	Lot.091M-5302V	1
Caelo	Sodium carbonate decahydrate	11254706	1
Caelo	Sodium carbonate decahydrate	11254708	1
Caelo	Sodium carbonate decahydrate	12239810	2
Caelo	Sodium carbonate decahydrate	80136179	1
Caelo	Sodium carbonate decahydrate	13036907	1
Caelo	Sodium carbonate decahydrate	13036909	1
Caelo	Sodium carbonate decahydrate	13036910	1
Caelo	Sodium carbonate decahydrate	13036902	2
Caelo	Sodium carbonate decahydrate	12239806	1
Caelo	Sodium carbonate decahydrate	80136428	1
Phönix	Sodium carbonate decahydrate	13036904	2
Audor Pharma	Sodium hyaluronate	AP30101305H	2
Audor Pharma	Sodium hyaluronate	AP30101404H	1
Audor Pharma	Sodium hyaluronate	A0397074	1
Audor Pharma	Sodium hyaluronate	AP30101505H	1
Audor Pharma	Sodium hyaluronate	AP30101404H	1
Caelo	Sodium hyaluronate	17234702	1
Caelo	Sodium hyaluronate	1263303	1
Caelo	Sodium hyaluronate	14188702	1
Caelo	Sodium hyaluronate	14364706	2
Caelo	Sodium hyaluronate	16246703	1
Caelo	Sodium hyaluronate	15204901	1
Caelo	Sodium hyaluronate	15204903	3
Caelo	Sodium hyaluronate	193031002	1
Caelo	Sodium hyaluronate	17234701	1
Caelo	Sodium hyaluronate	21002684002	4
Caelo	Sodium hyaluronate	15448803	1
Calo/AHD	Sodium hyaluronate	14364704	1
Euro OTC	Sodium hyaluronate	L1710023-02	3
Euro OTC	Sodium hyaluronate	L1907021-01	1
Euro OTC	Sodium hyaluronate	L1512025-01	2
Euro OTC	Sodium hyaluronate	L2103023-01	1
Fagron	Sodium hyaluronate	L1311012-01	1
Fisher Scientific	Sodium hyaluronate	A0387534	1
Caelo	Sodium hyaluronate	2100131002	1
Caelo	Sodium hyaluronate	21000131002	1
Alliance	Sodium hydrocarbonate	12324704	1
Fagron	Sodium hydrocarbonate	12G11-N03	7
Anzag/ Hedinger	Sodium hydrocarbonate	206027	1
Caelo	Sodium hydrocarbonate	11304813	1
Caelo	Sodium hydrocarbonate	8101203	1
Caelo	Sodium hydrocarbonate	12132204	7
Caelo	Sodium hydrocarbonate	12132219	8
Caelo	Sodium hydrocarbonate	1203030-1	1
Caelo	Sodium hydrocarbonate	12356303	3
Caelo	Sodium hydrocarbonate	12324725	1
Caelo	Sodium hydrocarbonate	12324708	1
Caelo	Sodium hydrocarbonate	12356401	4
Caelo	Sodium hydrocarbonate	13060117	1
Caelo	Sodium hydrocarbonate	13186704	1
Caelo	Sodium hydrocarbonate	12356403	1
Caelo	Sodium hydrocarbonate	12356407	2
Caelo	Sodium hydrocarbonate	13234004	2
Caelo	Sodium hydrocarbonate	6011404	1
Caelo	Sodium hydrocarbonate	13234005	4
Caelo	Sodium hydrocarbonate	13234007	4
Caelo	Sodium hydrocarbonate	13234202	3
Caelo	Sodium hydrocarbonate	13390520	1
Caelo	Sodium hydrocarbonate	13234205	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Sodium hydrocarbonate	12132503	1
Caelo	Sodium hydrocarbonate	15328602	1
Caelo	Sodium hydrocarbonate	13101706	1
Caelo	Sodium hydrocarbonate	11304802	2
Caelo	Sodium hydrocarbonate	13186706	2
Caelo	Sodium hydrocarbonate	1234702	2
Caelo	Sodium hydrocarbonate	12109204	3
Caelo	Sodium hydrocarbonate	13060103	8
Caelo	Sodium hydrocarbonate	3012Q-01892	1
Caelo	Sodium hydrocarbonate	13060120	5
Caelo	Sodium hydrocarbonate	13390505	1
Caelo	Sodium hydrocarbonate	13186721	1
Caelo	Sodium hydrocarbonate	11304809	1
Caelo	Sodium hydrocarbonate	12132203	3
Caelo	Sodium hydrocarbonate	1219204	1
Caesar & Loretz Gm…	Sodium hydrocarbonate	13060102	1
Eu Rho	Sodium hydrocarbonate	1203030-01	8
Euro OCT	Sodium hydrocarbonate	1307017-01	1
Euro OTC	Sodium hydrocarbonate	120303001	1
Euro OTC	Sodium hydrocarbonate	120800801	1
Euro OTC	Sodium hydrocarbonate	1012011-01	1
Euro OTC	Sodium hydrocarbonate	1109029-01	8
Euro OTC	Sodium hydrocarbonate	1012011	1
Euro OTC	Sodium hydrocarbonate	1208008-01	9
Euro OTC	Sodium hydrocarbonate	1304017-02	2
euroho/gehe	Sodium hydrocarbonate	123030-02	1
Euro OTC	Sodium hydrocarbonate	1104013-01	2
Euro OTC	Sodium hydrocarbonate	1304017-01	5
Fagron	Sodium hydrocarbonate	11K25-N05	3
Fagron	Sodium hydrocarbonate	12D11-No2	1
Fagron	Sodium hydrocarbonate	13D29-N09	4
Fagron	Sodium hydrocarbonate	11/12-N16	1
Fagron	Sodium hydrocarbonate	11I12-N16	3
Fagron	Sodium hydrocarbonate	12D11-N02	9
Fagron	Sodium hydrocarbonate	13G11-N03	2
Fagron	Sodium hydrocarbonate	RBA3421100	3
Fagron	Sodium hydrocarbonate	RBA3651200	1
Fagron	Sodium hydrocarbonate	4413I01892	1
Finze	Sodium hydrocarbonate	Pr.Nr.4311Q-01892	1
fischar	Sodium hydrocarbonate	6522101	6
Fischer/VDL	Sodium hydrocarbonate	6521111	5
Gehe	Sodium hydrocarbonate	11078315	1
Gehe	Sodium hydrocarbonate	1203030-02	8
Gehe	Sodium hydrocarbonate	12k09-N05	1
Caelo	Sodium hydrocarbonate	13186711	1
Phönix	Sodium hydrocarbonate	13186705	4
Phönix	Sodium hydrocarbonate	13390515	1
Caelo	Sodium hydrocarbonate	12324702	7
Caelo	Sodium hydrocarbonate	12109205	6
Fagron	Sodium hydrocarbonate	13B18-N03	6
Caelo	Sodium hydroxide	15312102	1
Caelo	Sodium hydroxide	11070821	1
Fagron	Sodium hydroxide	12E02-N15	1
Fagron	Sodium hydroxide	13F06-N02	3
Fagron	Sodium hydroxide	13k22-no5	1
Caelo	Sodium hydroxide	12368105	1
Caelo	Sodium methyl-4-hydroxybenzoate	17051903	2
Caelo	Sodium methyl-4-hydroxybenzoate	18060803	1
Caelo	Sodium methyl-4-hydroxybenzoate	18060801	1
Caelo	Sodium methyl-4-hydroxybenzoate	19143902	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Alliance healthcare	Sodium monohydrogenphosphat…	12L05-N04	2
Bombastus	Sodium monohydrogenphosphat…	11H04-N06	1
Fagron	Sodium monohydrogenphosphat…	613I-01914	1
Fagron	Sodium monohydrogenphosphat…	13D24-N12	2
Fagron	Sodium monohydrogenphosphat…	13H01-B01	1
AHD	Sodium monohydrogenphosphat…	112345013	1
Alliance	Sodium monohydrogenphosphat…	12256606	1
Caelo	Sodium monohydrogenphosphat…	1169315	1
Caelo	Sodium monohydrogenphosphat…	9302613	2
Caelo	Sodium monohydrogenphosphat…	11169315	1
Caelo	Sodium monohydrogenphosphat…	12345001	2
Caelo	Sodium monohydrogenphosphat…	12345004	7
Caelo	Sodium monohydrogenphosphat…	12345007	3
Caelo	Sodium monohydrogenphosphat…	12345013	6
Caelo	Sodium monohydrogenphosphat…	71199028	1
Caelo	Sodium monohydrogenphosphat…	12345016	7
Caelo	Sodium monohydrogenphosphat…	83002059	1
Caelo	Sodium monohydrogenphosphat…	12256602	2
Caelo	Sodium monohydrogenphosphat…	11169309	3
Caelo	Sodium monohydrogenphosphat…	11169303	2
Caelo	Sodium monohydrogenphosphat…	12345025	1
Caelo	Sodium monohydrogenphosphat…	AKD7	1
Caesar&loretz,Anzag	Sodium monohydrogenphosphat…	12256606	3
Fagron	Sodium monohydrogenphosphat…	11K30-N01	1
Fagron	Sodium monohydrogenphosphat…	2111E-01914	1
Fagron	Sodium monohydrogenphosphat…	1513I-01914	1
Fagron	Sodium monohydrogenphosphat…	B44888A	1
gebepharm	Sodium monohydrogenphosphat…	20160909-2	1
ICHTHYOL-GESELLSCHAFT	Sodium monohydrogenphosphat…	Caelo	1
Caelo	Sodium monohydrogenphosphat…	12109002	2
Caelo	Sodium monohydrogenphosphat…	12109106	1
Caelo	Sodium monohydrogenphosphat…	10135304	1
Caelo	Sodium monohydrogenphosphat…	12109109	1
Caelo	Sodium monohydrogenphosphat…	13028103	1
Caelo	Sodium monohydrogenphosphat…	11109513	1
Caelo	Sodium monohydrogenphosphat…	12109108	2
Caelo	Sodium monohydrogenphosphat…	13028001	1
Caelo	Sodium monohydrogenphosphat…	72006059	1
Gehe	Sodium monohydrogenphosphat…	12109001	2
Jenne	Sodium monohydrogenphosphat…	12109003	3
Phönix	Sodium monohydrogenphosphat…	1302800,	1
Phönix	Sodium monohydrogenphosphat…	13028101	1
Caelo	Sodium monohydrogenphosphat…	13028003	1
Caelo	Sodium perborate, hydrated	13050801	2
Caelo	Sodium perborate, hydrated	13050807	1
Caelo	Sodium perborate, hydrated	13050805	1
Aldrich	Sodium proprionate	U02796-056	1
Caelo	Sodium thiosulfate	80426288	1
Caelo	Sodium thiosulfate	26041302	1
Fagron	Sodium thiosulfate	13092013E	1
Fagron	Sodium thiosulfate	12F20-N20	1
Fagron	Sodium thiosulfate	12F20-N10	1
Fagron	Sodium thiosulfate	3313U-01922	1
Caelo	Softisan® 601	15184901	1
Caelo	Softisan® 601	13296104	1
Caelo	Softisan® 601	14099608	1
Caesar & Loretz GmbH	Softisan® 601	18197002	2
Caelo	Solanum dulcamara stems, cut	10375605	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Solanum dulcamara stems, cut	10375607	1
Caelo	Solanum dulcamara stems, cut	132564301	1
Caelo	Solanum dulcamara stems, cut	13254301	1
Caelo	Solanum dulcamara stems, cut	103745604	1
Klenk	Solanum dulcamara stems, cut	5601A080513	3
Caelo	Sorrel herb, cut	130546	1
Gahlke	Sorrel herb, cut	21479	1
Caelo	Sorrel herb, cut	13289502	2
Kräuter-Schulte	Sorrel herb, cut	55272	1
Caelo	Sour cherry stems, cut	10367019	1
Caelo	Sour cherry stems, cut	12042301	1
Caelo	Sour cherry stems, cut	10367014	1
Caelo	Sour cherry stems, cut	12042307	1
AHD	Spearmint leaf	14343404	1
Caelo	Spearmint leaf	12133901	3
Caelo	Spearmint leaf	1512Q-01505	1
Caelo	Spearmint leaf	11037409+110374	1
Caelo	Spearmint leaf	12133906	2
Caelo	Spearmint leaf	13105001	10
Caelo	Spearmint leaf	12376706	1
Caelo	Spearmint leaf	12133909	1
Caelo	Spearmint leaf	13105003	1
Anzag 12.03.13 ek:…	St. John's wort	11185608	2
Caelo	St. John's wort	12092201	1
Aurica	St. John's wort	521200778	1
Aurica	St. John's wort	521202559	1
Bahnhof-Apotheke	St. John's wort	4-121018	1
Bombastus	St. John's wort	268913	1
Bombastus	St. John's wort	275106	6
Bombastus	St. John's wort	265761	1
Bombastus	St. John's wort	268834	2
Caelo	St. John's wort	4021B110321	1
Caelo	St. John's wort	11185602	1
Caelo	St. John's wort	11185608	18
Caelo	St. John's wort	5021301	1
Caelo	St. John's wort	1185608	1
Caelo	St. John's wort	16041301	1
Caelo	St. John's wort	12092204	1
Caelo	St. John's wort	13091303	1
Caelo	St. John's wort	111185608	1
Caelo	St. John's wort	11185607	1
Caelo	St. John's wort	30011401	1
Caelo	St. John's wort	132203204	1
Caelo	St. John's wort	15068105	1
Caelo	St. John's wort	268913	1
Caelo	St. John's wort	13203204	6
Caelo	St. John's wort	13203205	1
Finze	St. John's wort	9297303	1
Galke	St. John's wort	21034	1
Galke	St. John's wort	21990	4
Galke	St. John's wort	23054	1
Galke	St. John's wort	21556	1
Gehe	St. John's wort	9297305	1
Gehe	St. John's wort	11185602	1
Bombastus	St. John's wort	281530	1
Hepart AG	St. John's wort	B-445,kbA	1
Klenk	St. John's wort	15068103	2
Klenk	St. John's wort	4021A100819	1
Klenk	St. John's wort	4021A100819	21
Klenk	St. John's wort	4021A100819914	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Klenk	St. John's wort	4021A100919	1
Klenk	St. John's wort	4021A-100819	1
Klenk	St. John's wort	A121120	1
Klenk	St. John's wort	4012A100819	1
Klenk	St. John's wort	A130612	3
Klenk	St. John's wort	4021A130612	4
Klenk	St. John's wort	4021a100819	1
Klenk	St. John's wort	4021a120604	1
Klenk	St. John's wort	4021B110321	2
Klenk	St. John's wort	4021A120604	16
Klenk	St. John's wort	4021A120905	9
Noweda	St. John's wort	12092202	6
Caelo	St. John's wort	12092209	2
Klenk	St. John's wort	4021A00819	1
Wolf	St. John's wort	206152	1
Wolf	St. John's wort	B206152	1
Wolf	St. John's wort	19468	2
Wolf	St. John's wort	B-455	2
Wolf	St. John's wort	B-424	1
Caelo	Star anise	10169101	1
Caelo	Star anise	10376403	2
Caelo	Star anise	11314104	1
Caelo	Star anise	12226211	1
Caelo	Star anise	10376405	1
Caelo	Star anise	11314103	1
Klenk	Star anise	2690A101026	1
Klenk	Star anise	2690A111013	3
Klenk	Star anise	2696B111109	1
Klenk	Star anise	B111109	1
Klenk	Star anise	2690A120809	1
Klenk	Star anise	2690A130903	2
Caelo	Star anise, cut	16253201	2
Caelo	Stemless carline root	23071203	1
Caelo	Stemless carline root	12144804	1
Caelo	Stemless carline root	13130303	1
Caelo	Stemless carline root	13033501	1
Caelo	Stemless carline root	25111306	1
Caelo	Stemless carline root	14347401	1
Caelo	Stemless carline root	13130301	6
Caelo	Stemless carline root	13130304	1
Caelo	Stemless carline root	12232803	1
Hepart AG	Stemless carline root	B120726	1
Klenk	Stemless carline root	12097301	1
Klenk	Stemless carline root	B110831	1
Klenk	Stemless carline root	6194b110831	1
Klenk	Stemless carline root	6194B110831	1
Klenk	Stemless carline root	6191B120726	3
Klenk	Stemless carline root	69191B120726	1
Nachprüfung	Stemless carline root	2812U02133	1
Noweda	Stemless carline root	12163702	1
Caelo	Strawberry leaf	11117909	1
Caelo	Strawberry leaf	5122013c	1
Klenk	Strawberry leaf	2031B110224	2
Klenk	Strawberry leaf	B120925	1
Klenk	Strawberry leaf	A130430	1
Klenk	Strawberry leaf	2031A130430	2
Caelo	Sulfamerazine	10218401	1
Fagron	Sulfanilamide	11L01-No8	1
Klenk	Sunflower, cut	1711I-07036	1
Klenk	Sunflower, cut	1701B091013	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Anzag	Sweet woodruff herb	12103504	2
Caelo	Sweet woodruff herb	10375802	1
Caelo	Sweet woodruff herb	4409M-01621	1
Caelo	Sweet woodruff herb	52236077	1
Caelo	Sweet woodruff herb	10375812	1
Caelo	Sweet woodruff herb	18031304	1
Caelo	Sweet woodruff herb	12103508	1
Caelo	Sweet woodruff herb	12103510	1
Caelo	Sweet woodruff herb	12103513	2
Caelo	Sweet woodruff herb	12103509	1
Caelo	Sweet woodruff herb	12103514	1
Gahlke	Sweet woodruff herb	22100	1
Klenk	Sweet woodruff herb	3601B090114	1
Klenk	Sweet woodruff herb	B090114	3
Klenk	Sweet woodruff herb	3601B140321	1
Kräuter-Schulte	Sweet woodruff herb	52878	1

T

Supplier	Substance	Batch	Spectra
Caelo	Talcum	11318324	4
Caelo	Talcum	28121201	1
Caelo	Talcum	11164313	1
Caelo	Talcum	11164306	1
Caelo	Talcum	12267401	4
Caelo	Talcum	9218303	1
Caelo	Talcum	12267412	7
Caelo	Talcum	11318312	2
Caelo	Talcum	15061301	1
Caelo	Talcum	13146301	1
Caelo	Talcum	13146308	6
Caelo	Talcum	13146307	3
Caelo	Talcum	13146312	4
Caelo	Talcum	2011406	1
Caelo	Talcum	13146316	3
Caelo	Talcum	13146315	1
Caelo	Talcum	12267424	5
Caelo	Talcum	12267423	3
Caelo	Talcum	11318311	3
Caelo	Talcum	11318335	4
Caelo	Talcum	13146302	8
Caelo	Talcum	11318301	1
EuRho	Talcum	1105024-02	1
Euro OTC	Talcum	1205046-01	2
Euro OTC	Talcum	1305022-01	7
Euro OTC	Talcum	1210052-01	4
Euro OTC	Talcum	1305022-02	1
Phönix	Talcum	10148805Retest	1
Caelo	Tall hawkweed, cut	3611b111005	1
Klenk	Tall hawkweed, cut	B111005	1
Klenk	Tall hawkweed, cut	3611B11105	1
Caelo	Tall nasturtium herb, cut	12031602	1
Caelo	Tall nasturtium herb, cut	12031601	1
Caelo	Tall nasturtium herb, cut	12031606	1
Caelo	Tall nasturtium herb, cut	12031603	1
Caelo	Tall nasturtium herb, cut	12031604	2
Caelo	Tall nasturtium herb, cut	13104401	4
Caelo	Tall nasturtium herb, cut	107063	1
Caelo	Tall nasturtium herb, cut	12031605	1
Caelo	Tall nasturtium herb, cut	13104402	2
Caelo	Tall nasturtium herb, cut	13104404	2

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tall nasturtium herb, cut	13104405	1
Caelo	Tall nasturtium herb, cut	13104403	5
Caelo	Tall nasturtium herb, cut	13104406	1
Caelo	Thalidomide	20081504	1
Fagron	Thalidomide	14E27-B04-299297	1
Fagron	Thalidomide	13K20-N01	1
Caelo	Theriac	12289301	4
Caelo	Theriac	11082413	1
Caelo	Theriac	2021301	1
Caelo	Theriac	15101307	1
Caelo	Theriac	412091-2P	1
Caelo	Theriac	12289312	1
Caelo	Theriac	13407304	2
Caelo	Theriac	15026401	3
Caelo	Theriac	11081515	1
Caelo	Theriac	15312501	2
Caelo	Theriac	1531501	1
Caelo	Theriac	15312511	2
Caelo	Theriac	14156501	1
Caelo	Theriac	12289307	8
Caelo	Theriac	12189404	2
Caelo	Theriac	12289305	2
Caelo	Theriac	15312508	1
Caelo	Theriac	12289303	1
Caelo	Theriac	12289306	1
Caelo	Theriac	15312504	1
Caelo	Theriac	12189401	1
Caesar/Noweda	Theriac	12289309	1
Klenk	Theriac	12189403	1
Aurica	Thyme	521207003	1
Bahnhof-Apotheke	Thyme	17-121112	1
Bombastus	Thyme	277996	2
Bombastus	Thyme	277466	1
Bombastus	Thyme	243485	1
Caelo	Thyme	10365807	2
Caelo	Thyme	10365816	1
Caelo	Thyme	8061206	1
Caelo	Thyme	11345004	4
Caelo	Thyme	15101201	1
Caelo	Thyme	12111201	1
Caelo	Thyme	11345007	5
Caelo	Thyme	21121204	1
Caelo	Thyme	11345001	1
Caelo	Thyme	11345010	6
Caelo	Thyme	29011303	1
Caelo	Thyme	11021301	1
Caelo	Thyme	22021301	1
Caelo	Thyme	23021304	1
Caelo	Thyme	26021301	1
Caelo	Thyme	4041301	1
Caelo	Thyme	11345014	12
Caelo	Thyme	25041302	1
Caelo	Thyme	11345013	9
Caelo	Thyme	1134514	1
Caelo	Thyme	13081301	1
Caelo	Thyme	25091304	1
Caelo	Thyme	29101301	1
Caelo	Thyme	11121306	1
Caelo	Thyme	13011402	1
Caelo	Thyme	13048308	2

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Thyme	16011401	1
Caelo	Thyme	4021512	1
Caelo	Thyme	13048314	1
Caelo	Thyme	14119001	1
Caelo	Thyme	15104401	1
Caelo	Thyme	11345002	1
Caelo	Thyme	11345006	3
Caelo	Thyme	13048302	2
Caelo	Thyme	13048301	14
Caelo	Thyme	13048309	4
Caelo	Thyme	10365815	2
Caelo	Thyme	11345011	13
Caelo	Thyme	13048309-3475312161	1
Euro OTC	Thyme	4622A130109	75
Galke	Thyme	19386	2
Galke	Thyme	28719	1
Galke	Thyme	20719	2
Galke	Thyme	1833	1
Gehe	Thyme	4622A110120	1
Klenk	Thyme	4622A110728	25
Klenk	Thyme	4622A120111	35
Hepart AG	Thyme	A130109	2
Klenk	Thyme	4622a110728	1
Klenk	Thyme	1910211688	1
Klenk	Thyme	4622a130109	2
Klenk	Thyme	4622A141203	1
Klenk	Thyme	4622B110519	1
Klenk	Thyme	2103311688	1
Klenk	Thyme	A130910	3
Klenk	Thyme	4622A130910	2
Klenk	Thyme	4622A12011	1
Klenk	Thyme	4622A-120111	1
Klenk	Thyme	4622A170207	1
Klenk	Thyme	4622A170905	3
Klenk	Thyme	4622a120111	3
Noweda	Thyme	521303908	1
Bombastus	Thyme	273909	3
Caelo	Thyme		1
Weltecke	Thyme	67101212	1
Caelo	Tonka beans	1078C	1
Caelo	Tonka beans	12145101	2
Caelo	Tonka beans	12144101	1
Caelo	Tonka beans	20111312	1
Noweda	Tonka beans	1040A111026	1
Aurica	Tormentil	521304332	1
Caelo	Tormentil	11102010	1
Caelo	Tormentil	12040704	2
Caelo	Tormentil	10081203	1
Caelo	Tormentil	2512A-02188	1
Caelo	Tormentil	12040717	1
Caelo	Tormentil	12216802	1
Caelo	Tormentil	12040707	1
Caelo	Tormentil	411082-2-P	1
Caelo	Tormentil	30011405	1
Caelo	Tormentil	25022014A	1
Caelo	Tormentil	14008005	1
Caelo	Tormentil	15085501	1
Caelo	Tormentil	14360103	1
Caelo	Tormentil	15178203	1
Caelo	Tormentil	15178206	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tormentil	15364316	1
Caelo	Tormentil	12216806	1
Caelo	Tormentil	14008001	2
Caelo	Tormentil	15364302	5
Caelo	Tormentil	4753268	1
Caelo	Tormentil	12040708	9
Caelo	Tormentil	12040713	1
Caelo	Tormentil	1914A-02188	1
Caelo	Tormentil	6911B140227	1
Caelo	Tormentil	14140001	1
Caelo	Tormentil	15178202	2
Caelo	Tormentil	12216803	4
Caelo	Tormentil	12216805	1
Caelo	Tormentil	14008002	2
Caelo	Tormentil	12216801	4
Cealo/Gehe	Tormentil	14140006	3
Galke	Tormentil	21091	1
Galke	Tormentil	21744	2
Caelo	Tormentil	13220502	1
Klenk	Tormentil	6911B131029	4
Klenk	Tormentil	6911B141114	2
Klenk	Tormentil	6911B150825	4
Klenk	Tormentil	6911B140227	1
Klenk	Tormentil	6911B111013	10
Klenk	Tormentil	6914b120112	1
kräuter schulte	Tormentil	51952	1
Noweda10.02.2017	Tormentil	15364313	3
phönix	Tormentil	15364343	1
Phönix	Tormentil	15364302	1
Richter	Tormentil	P209904	1
Sanacorp	Tormentil	12040712	3
AHD	Tragacanth	15379906	5
Caelo	Tragacanth	8081201	1
Caelo	Tragacanth	9081202	1
Caelo	Tragacanth	15121203	1
Caelo	Tragacanth	11128905	1
Caelo	Tragacanth	12285402	1
Caelo	Tragacanth	14011302	1
Caelo	Tragacanth	12285403	4
Caelo	Tragacanth	1228503	1
Caelo	Tragacanth	15041302	1
Caelo	Tragacanth	13095203	1
Caelo	Tragacanth	13095208	3
Caelo	Tragacanth	20111305	1
Caelo	Tragacanth	7021402	1
Caelo	Tragacanth	13277802	4
Caelo	Tragacanth	14162205	7
Caelo	Tragacanth	13204705	1
Caelo	Tragacanth	15085607	1
Caelo	Tragacanth	153799	1
Caelo	Tragacanth	16110802	2
Caelo	Tragacanth	14162207	1
Caelo	Tragacanth	15379907	1
Caelo	Tragacanth	14162207	2
Caelo	Tragacanth	13204701	4
Caelo	Tragacanth	15085606	7
Caelo	Tragacanth	13277804	4
Caelo	Tragacanth	15085602	1
Caelo	Tragacanth	12108806	1
Caelo	Tragacanth	1327802	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Tragacanth	12285408	1
Caelo	Tragacanth	16110807	3
Caelo	Tragacanth	16350004	1
Fagron	Tragacanth	13204705	5
JENNE	Tragacanth	16110801	1
Caelo	Tragacanth	15085602	4
Fagron	Triamcinolone acetonide 1:1…	12107-N04	1
Fagron	Triamcinolone acetonide 1:1…	11g14-n02	1
Fagron	Triamcinolone acetonide 1:1…	11G14-N02	1
Fagron	Triamcinolone acetonide 1:1…	13F21-N01	2
Fagron	Triamcinolone acetonide 1:1…	12F21-N01	1
Fagron	Triamcinolone acetonide 1:1…	14F17-N02	1
Fagron	Triamcinolone acetonide 1:1…	13A15-N05	1
Fagron	Triamcinolone acetonide 1:1…	13F20-N010113/150	1
Fagron	Triamcinolone acetonide 1:1…	12107-N04022/359	1
Fagron	Triamcinolone acetonide 1:1…	12I07-No4	1
Fagron	Triamcinolone acetonide 1:1…	12G23-N06	2
Fagron	Triamcinolone acetonide 1:1…	12I07-N04	1
Fargon/17.07.2013/…	Triamcinolone acetonide 1:1…	12|07-N04	1
Fagron	Triamcinolone acetonide 1:1…	12A05-N07	3
Fagron	Triamcinolone acetonide 1:1…	12E23-N01	2
Caelo	Tricalcium phosphate	1056303	1
EuRho	Tricalcium phosphate	13031203	1
Euro OTC	Tricalcium phosphate	1206002-01	3
Euro OTC	Tricalcium phosphate	1304025-01	2
Fagron	Tricalcium phosphate	12I13-N03	1
Anzag	Trichloroacetic acid	12135204	2
apomix	Trichloroacetic acid	12G04-M11	1
Caelo	Trichloroacetic acid	12135201	1
Caelo	Trichloroacetic acid	12g04m11	1
Caelo	Trichloroacetic acid	11294318	1
Caelo	Trichloroacetic acid	12135203	1
Caelo	Trichloroacetic acid	12135210	2
Caelo	Trichloroacetic acid	6091306	1
Caelo	Trichloroacetic acid	14101711	1
Caelo	Trichloroacetic acid	13056203	3
Caelo	Trichloroacetic acid	12135207	5
Caelo	Trichloroacetic acid	13056212	1
Caelo	Trichloroacetic acid	10379401	1
Caelo	Trichloroacetic acid	10130802	1
Fagron	Trichloroacetic acid	13B19-M04	1
Fagron	Trichloroacetic acid	13H22-M04	1
Merck	Trichloroacetic acid	12821	1
Caelo	Trichloroacetic acid	13056213	1
Caelo	Trichloroacetic acid	13056209	1
Caelo	Turmeric rhizome	12136504	1
Caelo	Turmeric rhizome	12136506	1
Caelo	Turmeric rhizome	12136507	1
Caelo	Turmeric rhizome	1213650	1
Caelo	Turmeric rhizome	13360204	2
Caelo	Turmeric rhizome	15158001	2
Caelo	Turmeric rhizome	15158001	2
Caelo	Turmeric rhizome	15372603	1
Caelo	Turmeric rhizome	16344604	2
Caelo	Turmeric rhizome	15207601	1
Caelo	Turmeric rhizome	12136501	2
Caelo	Turmeric rhizome	12136503	2
Galke	Turmeric rhizome	20184	1
Galke	Turmeric rhizome	23123	1
Klenk	Turmeric rhizome	6741B121030	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Turmeric, javanese	288629	1
Bombastus	Turmeric, javanese	262792	1
Bombastus	Turmeric, javanese	277130	1
Bombastus	Turmeric, javanese	282221	2
Bombastus	Turmeric, javanese	28221	1
Bombastus	Turmeric, javanese	284242	2
Caelo	Turmeric, javanese	25041313	1
Caelo	Turmeric, javanese	12319201	1
Caelo	Turmeric, javanese	13262907	1
Caelo	Turmeric, javanese	14309503	1
Caelo	Turmeric, javanese	15120202	3
Caelo	Turmeric, javanese	16094101	1
Caelo	Turmeric, javanese	14017706	1
Caelo	Turmeric, javanese	11182903	1
Caelo	Turmeric, javanese	17042002	1
Caelo	Turmeric, javanese	12319206	2
Caelo	Turmeric, javanese	17042003	1
Caelo	Turmeric, javanese	12319206	2
Galke	Turmeric, javanese	15540	1
Galke	Turmeric, javanese	15540	1
Klenk	Turmeric, javanese	6731B160426	1
Kenk / Phoenix	Turmeric, javanese	6731B130117	1
Klenk	Turmeric, javanese	B130117	1
Klenk	Turmeric, javanese	6731B150630	1
Noweda	Turmeric, javanese	6731B180412	1

U

Supplier	Substance	Batch	Spectra
Audor Pharma	Uridine	AP721060040/5U	3
Audor Pharma	Uridine	AP3015	1
Audor Pharma	Uridine	APIB1600182AU	8
Audor Pharma	Uridine	APIB1600169AU	44
Audor Pharma	Uridine	APIB1600169	2
Audor Pharma	Uridine	APIB1600169AU/Re	1
Audor Pharma	Uridine	AP30514U	5
Audor Pharma	Uridine	APIB1400280AU	1
Audor Pharma	Uridine	APIB1600182.11AU	1
Audor Pharma	Uridine	APIB16001169	1
Audor Pharma	Uridine	AP30514IB1500001AXU	5
Audor Pharma	Uridine	IB1600169AU	3
Caelo	Uridine	AP1600169AU	1
Caelo	Uridine	IB1600169A	1
Fagron	Uridine	11G07-N04	1
Fagron	Uridine	22041301	1
Fagron	Uridine	16101301	1
Fagron	Uridine	14051405	1
Fagron	Uridine	13D08-N26	1
Fagron	Uridine	721110090	4
Fagron	Uridine	12091402	1
Fagron	Uridine	APIB16000169au	1
Fagron	Uridine	13K18-B31	4
Fagron	Uridine	14F02-B09	1
Fagron	Uridine	13D29-N06	3
Fagron	Uridine	14F02-B09-305467	7
Phönix	Uridine	721010040	1
Roth / Roth	Uridine	410301476	1
siehe WE-Prüfprotokoll	Uridine	54/11	1

V

Supplier	Substance	Batch	Spectra
Klenk	Valerian root, cut	6641B120417	1
Aurica	Valerian root, cut	221838	2
Bombastus	Valerian root, cut	267863	1
Bombastus	Valerian root, cut	274722	1
Bombastus	Valerian root, cut	269457	1
Caelo	Valerian root, cut	12033812	8
Caelo	Valerian root, cut	11103601	1
Caelo	Valerian root, cut	11103602	1
Caelo	Valerian root, cut	11103608	1
Caelo	Valerian root, cut	11349101	4
Caelo	Valerian root, cut	11103612	2
Caelo	Valerian root, cut	3091202	1
Caelo	Valerian root, cut	11035002	1
Caelo	Valerian root, cut	31101202	1
Caelo	Valerian root, cut	11103607	3
Caelo	Valerian root, cut	31121201	1
Caelo	Valerian root, cut	12033805	4
Caelo	Valerian root, cut	2712A-02167	1
Caelo	Valerian root, cut	12033809	9
Caelo	Valerian root, cut	1203381	1
Caelo	Valerian root, cut	20081303	1
Caelo	Valerian root, cut	12033810	1
Caelo	Valerian root, cut	120338012	1
Caelo	Valerian root, cut	28101303	1
Caelo	Valerian root, cut	29101303	1
Caelo	Valerian root, cut	13287402	3
Caelo	Valerian root, cut	15175205	1
Caelo	Valerian root, cut	12033811	5
Caelo	Valerian root, cut	11103609	4
Caelo	Valerian root, cut	12033807	1
Caelo	Valerian root, cut	13119001	1
Caelo	Valerian root, cut	13119004	3
Caelo	Valerian root, cut	13119003	12
Caelo	Valerian root, cut	13196806	6
Caelo	Valerian root, cut	13196801-3564412081	1
Caelo	Valerian root, cut	13196802	4
Galke	Valerian root, cut	22070	1
Galke	Valerian root, cut	21798	4
Klenk	Valerian root, cut	13196808	1
Klenk	Valerian root, cut	6641B110317	2
Klenk	Valerian root, cut	6641B-110317	1
Klenk	Valerian root, cut	6641B100823	1
Klenk	Valerian root, cut	6645B130226	1
Klenk	Valerian root, cut	6641B130226	9
Caelo	Valerian root, cut	13119002	18
Caelo	Valerian root, cut	1319003	1
Sanacorp	Valerian root, cut	12033804	9
Caelo	Valerian root, cut	12033808	7
Berkel AHK	Valerian root, powdered	13287406	1
Berkel AHK	Valerian root, powdered	14179403	2
Caelo	Valerian root, powdered	13287402	2
Caelo	Valerian root, powdered	15175204	1
an	Verbena herb	12383007	1
Aurica	Verbena herb	521305668	1
Caelo	Verbena herb	11031106	5
Caelo	Verbena herb	11031108	5
Caelo	Verbena herb	11031103	1
Caelo	Verbena herb	11031110	6
Caelo	Verbena herb	19111205	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Verbena herb	12187601	15
Caelo	Verbena herb	12178601	1
Caelo	Verbena herb	12188203	6
Caelo	Verbena herb	4651b120611	1
Caelo	Verbena herb	13151001	18
Caelo	Verbena herb	12383002	2
Caelo	Verbena herb	6111301	1
Caelo	Verbena herb	12383005	1
Caelo	Verbena herb	13351401	1
Caelo	Verbena herb	15012405	1
Caelo	Verbena herb	11031105	2
Caelo	Verbena herb	12188202	14
Caelo	Verbena herb	2x12188202	1
Caelo	Verbena herb	13151003	5
Gehe	Verbena herb	4651B110310	2
Klenk	Verbena herb	4651A070828	3
Klenk	Verbena herb	4654B120611	1
Klenk	Verbena herb	A130923	1
Klenk	Verbena herb	4651B130611	2
Klenk	Verbena herb	4651B120611	17
Caelo	Verbena herb	110031110	1

W

Supplier	Substance	Batch	Spectra
Bombastus	Walnut bark	711B1206130	1
Caelo	Walnut bark	11016604	1
Caelo	Walnut bark	11325606	2
Caelo	Walnut bark	11325605	1
Caelo	Walnut bark	11016605	1
Caelo	Walnut bark	11325603	1
Fiebig 16.11.12 ek:2,35	Walnut bark	711B111020	5
Gehe	Walnut bark	711B110128	3
Klenk	Walnut bark	711B120613	3
Klenk	Walnut bark	711B080806	1
Klenk	Walnut bark	711b120613	1
Klenk	Walnut bark	711B120906	2
ANZAG	Walnut leaf	12124603	15
Anzag ek: 4,58EUR 25...	Walnut leaf	2111A120123	9
Caelo	Walnut leaf	11103010	5
ApoFit/Noweda	Walnut leaf	271137	1
Caelo	Walnut leaf	10050416	1
Caelo	Walnut leaf	11103003	2
Caelo	Walnut leaf	11103004	2
Caelo	Walnut leaf	11103007	6
Caelo	Walnut leaf	11103008	5
Caelo	Walnut leaf	3051301	1
Caelo	Walnut leaf	1214603	1
Caelo	Walnut leaf	11103001	1
Caelo	Walnut leaf	12124602	3
Caelo	Walnut leaf	25041404	1
Caelo	Walnut leaf	12124502	1
Caelo	Walnut leaf	14064903	1
Caelo	Walnut leaf	14064906	3
Caelo	Walnut leaf	8071502	1
Caelo	Walnut leaf	15126004	1
Caelo	Walnut leaf	15126003	6
Caelo	Walnut leaf	1005903	1
Caelo	Walnut leaf	12124601	8
Caelo	Walnut leaf	16044002	4

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	Walnut leaf	16044008	1
Caelo	Walnut leaf	15126002	1
Caelo	Walnut leaf	3712Q-01499	1
Caelo	Walnut leaf	12124603-341930192	1
Caelo	Walnut leaf	1414Q01499	1
Caelo	Walnut leaf	14064909	2
Caelo	Walnut leaf	14064910	1
Caelo	Walnut leaf	14064902	5
Caelo	Walnut leaf	4713U01499	1
Caelo	Walnut leaf	414Q1499	1
Caelo	Walnut leaf	12124605	8
Caelo	Walnut leaf	14064904	4
Caelo	Walnut leaf	15126008	6
Galke	Walnut leaf	21061	1
Gehe	Walnut leaf	10050412	1
Gehe	Walnut leaf	2111B151028	3
Hepart AG	Walnut leaf	A120123	1
Caelo	Walnut leaf	11103009	1
Klenk	Walnut leaf	2111A110816	1
Klenk	Walnut leaf	F-280513-1	1
Klenk	Walnut leaf	A130410	1
Klenk	Walnut leaf	2111A131029	1
Klenk	Walnut leaf	2111A130410	4
Klenk	Walnut leaf	2111A-120123	1
Klenk	Walnut leaf	211B151028	1
noweda	Walnut leaf		1
Caelo	White deadnettle flower	10081206	1
Caelo	White deadnettle flower	12152402	2
Caelo	White deadnettle flower	11371610	5
Caelo	White deadnettle flower	11371609	3
Caelo	White deadnettle flower	2101301	1
Caelo	White deadnettle flower	11371613	2
Caelo	White deadnettle flower	15299101	1
Caelo	White deadnettle flower	52470437	1
Galke	White deadnettle flower	21691	4
Galke	White deadnettle flower	22704	1
Klenk	White deadnettle flower	1470A120111	4
Caelo	White deadnettle flower	11371611	2
Caelo	White deadnettle flower	12275802	1
Klenk	White deadnettle flower	1470A080103	1
Caelo	White deadnettle herb	11371702	1
Caelo	White deadnettle herb	11371706	3
Caelo	White deadnettle herb	11371709	2
Caelo	White deadnettle herb	11371711	2
Caelo	White deadnettle herb	11371705	1
Caelo	White deadnettle herb	11371712	1
Caelo	White deadnettle herb	11371703	1
Galke	White deadnettle herb	22253	2
Galke	White deadnettle herb	19706	1
Caelo	White mustard seed	15120304	1
Caelo	White mustard seed, powdered	7254a110823	1
Caelo	White mustard seed, powdered	12375701	1
Caelo	White mustard seed, powdered	12375705	1
Caelo	White mustard seed, powdered	12375706	2
Caelo	White mustard seed, powdered	12375704	1
Caelo	White mustard seed, powdered	12375705	4
Caelo	White mustard seed, powdered	13224804	3
Caelo	White mustard seed, powdered	13224801	1
Caelo	White mustard seed, powdered	12375702	1
Klenk	White mustard seed, powdered	7254A141202	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Caelo	White mustard seed, powdered	11114409	1
Caelo	Wild apple, sweet	11229805	1
Bombastus	Wild pansy	276259	3
Bombastus	Wild pansy	280890	1
Bombastus	Wild pansy	274237	2
Bombastus	Wild pansy	272832	1
Bombastus	Wild pansy	278106	2
Bombastus	Wild pansy	279314	3
Bombastus	Wild pansy	282661	2
Bombastus	Wild pansy	278106	2
Bombastus	Wild pansy	220232	1
Caelo	Wild pansy	10291007	1
Caelo	Wild pansy	13091205	1
Caelo	Wild pansy	10291009	3
Caelo	Wild pansy	17101205	1
Caelo	Wild pansy	5021304	1
Caelo	Wild pansy	15021301	1
Caelo	Wild pansy	11216103	2
Caelo	Wild pansy	12189203	4
Caelo	Wild pansy	14061311	1
Caelo	Wild pansy	7101303	1
Caelo	Wild pansy	12382806	1
Caelo	Wild pansy	12189204	4
Caelo	Wild pansy	12189204	10
Caelo	Wild pansy	4681A180411	1
Caelo	Wild pansy	12189204-3458312120	1
Caelo	Wild pansy	1289203	1
Caelo	Wild pansy	12189203	5
Caelo	Wild pansy	12382802	1
Caelo	Wild pansy	12189204-3463312101	1
Fagron	Wild pansy		1
Gehe	Wild pansy	11216103	3
Klenk	Wild pansy	4681A110303	2
Klenk	Wild pansy	4681A120806	1
Klenk	Wild pansy	B130715	1
Klenk	Wild pansy	4681B130715	5
Klenk	Wild pansy	4681A181105	1
Klenk	Wild pansy	4681A-120806	1
Klenk	Wild pansy	4681A120806	15
Nachprüfung	Wild pansy	10291007	1
Sanacorp	Wild pansy	12221-01694	1
-	Wild thyme, cut	131023	1
-	Wild thyme, cut	130685	1
Caelo	Wild thyme, cut	11031203	1
Caelo	Wild thyme, cut	11374805	5
Caelo	Wild thyme, cut	11374805i.O.	1
Caelo	Wild thyme, cut	4501A120813	2
Caelo	Wild thyme, cut	13086805	3
Caelo	Wild thyme, cut	11374803	1
Caesar & Loretz Gm...	Wild thyme, cut	11374802	1
Finze	Wild thyme, cut	11031204	1
Gehe	Wild thyme, cut	1090413	1
vedono	Wild thyme, cut	11374807	2
Bomba/AHD	Willow bark	280362	1
Bombastus	Willow bark	261615	1
Bombastus	Willow bark	277005	3
Bombastus	Willow bark	278458	2
Bombastus	Willow bark	277847	1
Bombastus	Willow bark	288869	1
Bombastus	Willow bark	251385	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Bombastus	Willow bark	292710	1
Bombastus	Willow bark	282270	1
Bombastus	Willow bark	281533	2
Bombastus	Willow bark	161594	1
Caelo	Willow bark	11073210	3
Caelo	Willow bark	11073201	1
Caelo	Willow bark	12185201	5
Caelo	Willow bark	21011302	1
Caelo	Willow bark	12185206	5
Caelo	Willow bark	11073208	1
Caelo	Willow bark	2185206	1
Caelo	Willow bark	12185208	12
Caelo	Willow bark	9071301	1
Caelo	Willow bark	13180702	4
Caelo	Willow bark	13180705	1
Caelo	Willow bark	12185204	4
Caelo	Willow bark	12185207	3
Caelo	Willow bark	13180701	1
Caelo	Willow bark	13180705-3530411072	1
Galke	Willow bark	20338	1
Klenk	Willow bark	811B100910	3
Klenk	Willow bark	B100910	6
Noweda	Willow bark	4609A-01305	1
Caelo	Willow herb	11347318	2
Caelo	Willow herb	11347311	1
Caelo	Willow herb	13104702	1
Caelo	Willow herb	11347316	1
Caelo	Willow herb	13200203	1
Caelo	Willowherb, small flowered	12064506	1
Bahnhof-Apotheke	Willowherb, small flowered	17-121107	1
Bombastus	Willowherb, small flowered	281846	2
Caelo	Willowherb, small flowered	7071201	1
Caelo	Willowherb, small flowered	9378908	1
Caelo	Willowherb, small flowered	29121201	1
Caelo	Willowherb, small flowered	2412E-01641	1
Caelo	Willowherb, small flowered	1031301	1
Caelo	Willowherb, small flowered	18031305	1
Caelo	Willowherb, small flowered	28031318	1
Caelo	Willowherb, small flowered	12041301	1
Caelo	Willowherb, small flowered	21061307	1
Caelo	Willowherb, small flowered	13071301	1
Caelo	Willowherb, small flowered	10326107	1
Caelo	Willowherb, small flowered	2081305	1
Caelo	Willowherb, small flowered	412041	1
Caelo	Willowherb, small flowered	16081302	1
Caelo	Willowherb, small flowered	16081304	1
Caelo	Willowherb, small flowered	15101302	1
Caelo	Willowherb, small flowered	13200203	7
Caelo	Willowherb, small flowered	31101303	1
Caelo	Willowherb, small flowered	15011411	1
Caelo	Willowherb, small flowered	13355906	2
Caelo	Willowherb, small flowered	14267909	1
Caelo	Willowherb, small flowered	10326104	5
Caelo	Willowherb, small flowered	13200201	3
Caelo	Willowherb, small flowered	13200202-3481312102	1
Caelo	Willowherb, small flowered	10326108	14
Caelo	Willowherb, small flowered	12117701-3371319012	1
Galke	Willowherb, small flowered	47502	1
Galke	Willowherb, small flowered	22347	4
Klenk	Willowherb, small flowered	4721C2120321	1

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Hepart AG	Willowherb, small flowered	10326110	2
Klenk	Willowherb, small flowered	C120321	1
Klenk	Willowherb, small flowered	A120418	1
Klenk	Willowherb, small flowered	4721B130528	1
Klenk	Willowherb, small flowered	4721A101010	2
Klenk	Willowherb, small flowered	4721C120321	10
Klenk	Willowherb, small flowered	4721A120418	11
Klenk	Willowherb, small flowered	4721C110701	4
Klenk	Willowherb, small flowered	4721C130618	4
Klenk	Willowherb, small flowered	4721A120903	7
Klenk	Willowherb, small flowered	2512U-01641	1
Caelo	Willowherb, small flowered	12117701	8
Bahnhof-Apotheke	Wormwood	17-121107	1
Bombastus	Wormwood	281000	1
Bombastus	Wormwood	265417	2
Bombastus	Wormwood	221868	1
Caelo	Wormwood	11285802	2
Caelo	Wormwood	11285810	6
Caelo	Wormwood	6101203	1
Caelo	Wormwood	12355801	20
Caelo	Wormwood	7031301	1
Caelo	Wormwood	12355807	10
Caelo	Wormwood	13174401	3
Caelo	Wormwood	7011401	1
Caelo	Wormwood	13381902	3
Caelo	Wormwood	13381905	1
Caelo	Wormwood	15408304	1
Caelo	Wormwood	13174402	2
Caelo	Wormwood	11285805	2
Caelo	Wormwood	12355804	8
Caelo	Wormwood	12355802	3
Caelo	Wormwood	12355805	4
Caelo	Wormwood	12355808	2
Caelo	Wormwood	11285803	1
Caelo	Wormwood	272957	1
Caelo	Wormwood	277513	1
Galke	Wormwood	21330	1
Gehe	Wormwood	11285811	1
Gehe	Wormwood	13381901	1
Klenk	Wormwood	3461A121130	2
Klenk	Wormwood	3461A110324	2
Klenk	Wormwood	A110324	1
Klenk	Wormwood	3461A1100324	1
Phoenix	Wormwood	12103003	8
Phönix	Wormwood	12355806	7
Sanacorp	Wormwood	12103002	2
Caelo	Wormwood	12355803	27

Y

Supplier	Substance	Batch	Spectra
Klenk	Yarrow flower	4181A121130	1
Caelo	Yarrow flower	12267702	1
Caelo	Yarrow flower	12363005	5
Caelo	Yarrow flower	13350507	1
Caelo	Yarrow flower	12267703	2
Caelo	Yarrow flower	12363002	6
Caelo	Yarrow flower	12338306	1
Caelo	Yarrow flower	70139427	1
Klenk	Yarrow flower	A110816	3
Alfred Galke	Yarrow herb	19861	1

continued on the next page

continued from previous page

Supplier	Substance	Batch	Spectra
Anzag 12.11.12 ek:3,85	Yarrow herb	11280513	1
Bahnhof-Apotheke	Yarrow herb	7-121011	1
Bombastus	Yarrow herb	274610	2
Bombastus	Yarrow herb	276498	1
Bombastus	Yarrow herb	274284	1
Bombastus	Yarrow herb	15006702	1
Bombastus	Yarrow herb	275964	1
Caelo	Yarrow herb	10101205	1
Caelo	Yarrow herb	11218404	1
Caelo	Yarrow herb	11280517	1
Caelo	Yarrow herb	11280511	2
Caelo	Yarrow herb	11306301	1
Caelo	Yarrow herb	12338304	15
Caelo	Yarrow herb	12338305	7
Caelo	Yarrow herb	5021302	1
Caelo	Yarrow herb	12379602	9
Caelo	Yarrow herb	12379603	7
Caelo	Yarrow herb	12338311	2
Caelo	Yarrow herb	12041302	1
Caelo	Yarrow herb	16041302	1
Caelo	Yarrow herb	H-220313-1	1
Caelo	Yarrow herb	13029104	5
Caelo	Yarrow herb	29071301	1
Caelo	Yarrow herb	10081301	1
Caelo	Yarrow herb	13029106	10
Caelo	Yarrow herb	13029105	4
Caelo	Yarrow herb	9101311	1
Caelo	Yarrow herb	16102013E	1
Caelo	Yarrow herb	12379606	9
Caelo	Yarrow herb	9121304	1
Caelo	Yarrow herb	12379607	1
Caelo	Yarrow herb	8011421	1
Caelo	Yarrow herb	27011404	1
Caelo	Yarrow herb	13381810	1
Caelo	Yarrow herb	13381805	1
Caelo	Yarrow herb	14018503	2
Caelo	Yarrow herb	1408510	1
Caelo	Yarrow herb	15006713	1
Caelo	Yarrow herb	15006720	1
Caelo	Yarrow herb	15006708	1
Caelo	Yarrow herb	13029108	9
Caelo	Yarrow herb	12336306	1
Caelo	Yarrow herb	13029103	13
Caelo	Yarrow herb	11280514	2
Caelo	Yarrow herb	12338306-3358319071	1
Caelo	Yarrow herb	1309106	1
Caelo	Yarrow herb	11280512	9
Caelo	Yarrow herb	18304002	1
Caelo	Yarrow herb	18304016	1
Caelo	Yarrow herb	18088002	1
Caelo	Yarrow herb	18304013	1
Caelo	Yarrow herb	12338303	10
Caelo	Yarrow herb	12379601	9
Caelo	Yarrow herb	13029107-3418310182	1
Caelo	Yarrow herb	13029107-3436311151	1
Caelo	Yarrow herb	13381806	2
Caelo	Yarrow herb	130929105	1
Caesar & Lorenz	Yarrow herb	12379605	3
Caesar & Loretz Gm…	Yarrow herb	11306303	1
Caesar & Loretz Gm…	Yarrow herb	12338306	3

continued on the next page

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

continued from previous page

Supplier	Substance	Batch	Spectra
Fagron	Yarrow herb	3613M-0165	1
Galke	Yarrow herb	21295	2
Galke	Yarrow herb	22048	7
Galke	Yarrow herb	23318	1
Galke	Yarrow herb	23735	1
Gehe	Yarrow herb	1128503	1
Gehe	Yarrow herb	4181A111122	5
Gehe	Yarrow herb	279023	3
Klenk	Yarrow herb	15333007	1
Klenk	Yarrow herb	4181A101102	1
Klenk	Yarrow herb	4181A110111	16
Klenk	Yarrow herb	A130709	1
Klenk	Yarrow herb	4181A130710	1
Klenk	Yarrow herb	4181130709	1
Klenk	Yarrow herb	4181B130709	2
Klenk	Yarrow herb	4181a11011	1
Klenk	Yarrow herb	4181a130513	1
Klenk	Yarrow herb	4181A121130	12
nachprüfung	Yarrow herb	C1320	1
Noweda	Yarrow herb	12378603	1
Noweda	Yarrow herb	13381804	2
Phagron	Yarrow herb		3
Caelo	Yarrow herb	18088008	1
Phönix	Yarrow herb	4181A130513	10
Wolf	Yarrow herb	230010	1
Wolf	Yarrow herb	B230010	9
Caelo	Yellow chaste weed	1024407	1
Caelo	Yellow chaste weed	10244407	1
Caelo	Yellow chaste weed	12170605	2
Caelo	Yellow chaste weed	15029505	1
Caelo	Yellow chaste weed	11293101	4
Caelo	Yellow chaste weed	512U-01473	1
Caelo	Yellow chaste weed	12170603	1
Klenk	Yellow chaste weed	1591A110511	13
Klenk	Yellow chaste weed	1591A-110511	1
Caelo	Yellow chaste weed	12170602	2
VDL	Yellow chaste weed	10244406	1

Z

Supplier	Substance	Batch	Spectra
Caelo	Zedoary root	11091603	1
Caelo	Zedoary root	13010104	1
Caelo	Zedoary root	25111304	1
Caelo	Zedoary root	12125301	3
Caelo	Zedoary root	13010102	3
Caelo	Zedoary root	12125304	2
Klenk	Zedoary root	6941B121025	3
Klenk	Zedoary root	6941B110329	2
Noweda	Zedoary root	11091605	3
Caelo	Zedoary root	111091607	1
vedono	Zedoary root	13010106	3
Caelo	Zedoary root, powdered	12007504	1
Caelo	Zedoary root, powdered	13165501	2
Caelo	Zedoary root, powdered	13165504	4
Caelo	Zedoary root, powdered	15277101	1
Caelo	Zedoary root, powdered	15352606	1
Klenk	Zedoary root, powdered	12007505	1

Appendix D: Requirements of validation

In order to ensure adherence to the safe scientific status, the individual methods for manufacturing and testing must be validated under certain circumstances (compare § 34 para. 1 no. 3, § 35 para. 1 no. 4 and para. 4 sentence 1 no. 2 b, para. 6 sentence 3 *ApoBetrO* [Pharmacies Rules and Regulations]). The *ApoBetrO* [Pharmacies Rules and Regulations] incorporates a legal definition in § 1 a para. 16 (quotation translated):

> *"Validation is the provision of documented proof which with a high degree of safety documents that, via a specific process or standard work process, a medicinal product is manufactured and tested, which is in accordance with previously determined quality features."*

Validation documentation can be used to prove that methods or devices which are not described in the Pharmacopoeia within the meaning of § 6 para. 1 sentence 3 *ApBetrO* [Pharmacies Rules and Regulations] achieve the same results as those in the Pharmacopoeia. On the other hand, with the requirements of the demanded validation it must be observed whether the respective testing method is already incorporated in the Pharmacopoeia.

NIR spectroscopy as a general testing method need not be validated in accordance with the express ruling in the *Ph. Eur. Section 1.1* [3], as it is already described in *Section 2.2.40* of the *Ph. Eur.* as an area of application for the identification of raw materials.

However, a special validation requirement exists for the reference database. This requirement is met with the existing document. Further requirements or rules as to how this proof must be furnished do not exist. It is required that the processes guarantee the same results as the methods and devices in the Pharmacopoeia [17].

Carrying out identity tests with *Apo-Ident* is therefore also possible if the NIR spectroscopy process is not required in the Pharmacopoeia monograph of the substance for identity testing. All NIR analyses with *Apo-Ident* prove several, often all molecule groups and are therefore comparable with a series of individual, targeted chemical proofs [4]. Therefore, the identity proof with *Apo-Ident* replaces the monograph test series (with two or more test combinations).

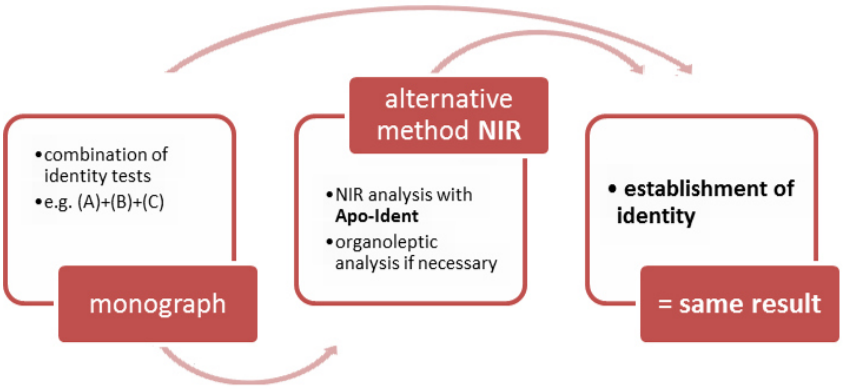


Figure 2: The combination of tests of the monograph is replaced by the alternative method NIR spectroscopy using *Apo-Ident*. This is permissible because both test procedures result in the establishment of the identity of the raw material.

With this validation documentation, proof is furnished that identical results are achieved with *Apo-Ident* and Pharmacopoeia methods, i.e. confirmation of the identity of the raw material [2].

Appendix E: Conformity of *Apo-Ident* with the *European pharmacopeia*

According to *Ph. Eur. Section 2.2.40*, NIR spectroscopy is basically suitable for: "Identification of agents, excipients, dosage forms, intermediate manufacturing products, chemical raw materials and packaging materials" ([3], quotation translated).

The fact that *Apo-Ident* meets the further criteria of the European Pharmacopoeia under the headings in *Section 2.2.40*

- Apparatus
- Measurement methods
- Sample preparation and presentation
- Testing the functionality of the instrument
- Identification and characterisation (qualitative analysis)
- Quantitative analysis
- Ongoing model evaluation
- Transfer of databases
- Data storage

can be proven based on the *HiperScan GmbH* documentation of "Meeting *2.2.40 Ph. Eur.* by *Apo-Ident*" [4].

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Appendix F: Addition to the second-stage models

As described in the general part of the *Apo-Ident* validation documentation, in the section Model creation procedure and validation runs, under *2. Generating the chemometric models (calibration)* in *f)*, it is possible to create a further chemometric model for certain substances (second-stage model) and to undertake the assessment in several steps.

Substances in second-stage models

In the substance class *APIs & excipients, solid*, a distinction is made between the following substances in the listed second-stage models:

Submodell - Submodel 01

Beeswax, white
Beeswax, yellow
Cetyl palmitate
Cocoa butter
Hard fat
Hard fat W35
Magnesium stearate
Paraffin, hard
Paraffin, microcrystalline
Sodium dodecyl sulfate

Submodell - Submodel 02

Betamethasone
Dexamethasone
Fluocinolone acetonide
Gramicidin
Methylprednisolone
Prednisolone
Triamcinolone acetonide
Tyrothricin

Submodell - Submodel 03

Acacia, dried dispersion
alpha-tocopheryl acetate dry concentrate
Amphotericin B
Bacitracin
Calcium glycerophosphate
Calcium pantothenate
Carmellose sodium
Cholecalciferol dry concentrate
Colistin sulfate
Corn starch
Cyanocobalamin
Erythromycin lactobionate
Estradiol hemihydrate
Estriol
Eucalyptus leaf
Fructose
Gelatine, white
Hyoscine hydrobromide

Maltodextrin
Methylcobalamin
Nystatin
Oxalic acid
Polymyxin B sulfate
Potato starch
Riboflavin
Rice starch
Selenium yeast
SyrSpend® SF Alka
SyrSpend® SF pH4
SyrSpend® SF pH4 neo (Maize starch)
Tosylchloramide sodium
Triamcinolone
Wheat starch

Submodell - Submodel 04

Carbomers
Finasteride
Gentamicin sulfate
Magnesium citrate
Mg-Ca-K colamine phosphate
Neomycin sulfate
Riboflavin sodium phosphate hydrate
Sodium tetraborate
Tobramycin sulfate
Zinc gluconate

Submodell - Submodel 05

Fusidic acid
Povidone
Povidone iodine
Progesterone
Spironolactone
Testosterone propionate
Ubidecarenone

Submodell - Submodel 07

Betamethasone valerate
Budesonide
Erythromycin

Submodell - Submodel 08

Ephedrine hydrochloride
Prednisolone acetate
Prednisone

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Submodell - Submodel 09

Acetylsalicylic acid
Benzoic acid
Dequalinium chloride
Dithranol
Eosin Y
Levothyroxin sodium
Oxytetracycline hydrochloride
Sodium salicylate
Tannin

Submodell - Submodel 12

Clioquinol
Mesalazine
Miconazole nitrate
Nicotinic acid
Theophylline-ethylenediamine hydrate

Submodell - Submodel 13

Alfatradiol
Amifampridine
Amitriptyline hydrochloride
Capsaicin
Ciprofloxacin hydrochloride
Cyproterone acetate
Heparin sodium
Levocarnitine
Methoxsalen
Norethisterone acetate
Oxybutynin hydrochloride
Prednicarbate
Pyridoxal-5-phosphate
Quinine hydrochloride dihydrate
Sodium citrate
Sucrose
Tetracaine
Triclosan
Valine

Submodell - Submodel 14

Atropine sulfate
Calcium orotate dihydrate
Escin, water-soluble
Hydrocortisone
Magnesium hydrogen citrate
Mometasone furoate
Phenytoin
Potassium sorbate
Propranolol hydrochloride
Quinoline yellow
Saccharin sodium

Submodell - Submodel 15

Beclometasone dipropionate
Betamethasone dipropionate
Clobetasol propionate

Submodell - Submodel 18

Diphenylcyclopropenone
Sodium benzoate

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

References

[1] ABDA – Bundesvereinigung Deutscher Apothekerverbände: Verordnung über den Betrieb von Apotheken (Apothekenbetriebsordnung – ApBetrO), 2012

[2] Reimann, B. ; Regierungspräsidium Darmstadt: Hinweise zur ordnungsgemäßen Prüfung von Arzneimitteln und Ausgangsstoffen (§§ 6 und 11 *ApBetrO*), 2007

[3] *Europäisches Arzneibuch, Implementation 2022*. 11. Edition. Deutscher Apotheker Verlag (978-3-7692-8026-5)

[4] HiperScan GmbH: Erfüllung von 2.2.40 Ph. Eur. durch Apo-Ident, 2013

[5] Arbeitsgemeinschaft der Pharmazieräte Deutschlands (APD): Resolution in Verbindung mit §§ 6 und 11 *ApBetrO* Verwendung eines Nah-Infrarot-Spektrometers (NIR) zur Identitätsprüfung, 16. 10. 2013, DAZ 48, November 2013

[6] Arbeitsgemeinschaft der Pharmazieräte Deutschlands (APD): Resolution 2014, Arbeitsgemeinschaft der Pharmazieräte Deutschlands (APD), Oktober 2014

[7] *DAC/NRF*. Govi-Verlag (978-3-7741-0044-2)

[8] Kessler, W.: *Multivariate Datenanalyse*. WILEY-VCH Verlag, 2007 (978-3-527-31262-7)

[9] Næs, T. ; Isaksson, T. ; Fearn, T. ; Davies, T.: *Multivariate Calibration and Classification*. NIR Publications, 2002 (978 0 9528666 2 6)

[10] Hanley, J. A. ; Lippman-Hand, A.: If nothing goes wrong, is everything all right? In: *Journal of the American Medical Association* 249 (1983), S. 1743–1745

[11] Jovanovic, B. D. ; Levy, P. S.: A Look at the Rule of Three. In: *The American Statistician* 51 (1997), S. 137–139

[12] Bronstein, I. N. ; Semendjajew, K. A. ; Musiol, G. ; Mühlig, H.: *Taschenbuch der Mathematik*. 5. überarbeitete und erweiterte Auflage. Verlag Harri Deutsch, 2000 (3-8171-2015-2)

[13] Mahalanobis, P.: On the generalized distance in statistics. In: *Proc. Nat. Inst. Sci. India (Calcutta)* 2 (1936), S. 49–55

[14] Yambor, B. ; Draper, W. ; Beveridge, R.: Analyzing PCA-based face recognition algorithms: Eigenvector selection and distance measures. In: *Second Workshop Empirical Evaluation in Computer Vision* (2000)

[15] HiperScan GmbH: Identifikationsmethodik Apo-Ident, 2012

[16] HiperScan GmbH: Datenvorbehandlung des Identifikationssystems Apo-Ident, 2012

[17] Cyran ; Rotta: Apothekenbetriebsordnung, Kommentar § 6 Rn. 10, 2010

Index

4-Aminobenzoic acid, 25
5-aminolevulinic acid hydrochloride, 29

L-Leucine, *see* Leucine, 1381

Acacia, dried dispersion, 35
Acaciae gummi dispersione desiccatum, *see* Acacia, dried dispersion, 35
Acetylcysteine, 41
Acetylcysteinum, *see* Acetylcysteine, 41
Acetylsalicylic acid, 47
Aciclovir, 55
Aciclovirum, *see* Aciclovir, 55
Acidum 4-aminobenzoicum, *see* 4-Aminobenzoic acid, 25
Acidum acetylsalicylicum, *see* Acetylsalicylic acid, 47
Acidum aminolaevulinicum hydrochloricum, *see* 5-aminolevulinic acid hydrochloride, 29
Acidum ascorbicum, *see* Ascorbic acid, 173
Acidum asparticum, *see* Aspartic acid, 191
Acidum benzoicum, *see* Benzoic acid, 231
Acidum boricum, *see* Boric acid, 323
Acidum citricum, *see* Citric acid, 593
Acidum citricum monohydricum, *see* Citric acid monohydrate, 617
Acidum folicum hydricum, *see* Folic acid hydrate, 1037
Acidum fusidicum, *see* Fusidic acid, 1063
Acidum glutaminicum, *see* Glutamic acid, 1137
Acidum nicotinicum, *see* Nicotinic acid, 1851
Acidum oxalicum cryst., *see* Oxalic acid, 1939
Acidum salicylicum, *see* Salicylic acid, 2355
Acidum sorbicum, *see* Sorbic acid, 2499
Acidum stearicum, *see* Stearic acid 50, 2555
Acidum tartaricum, *see* Tartaric acid, 2619
Acidum tranexamicum, *see* Tranexamic acid, 2735
Acidum ursodeoxycholicum, *see* Ursodeoxycholic acid, 2893
Adeps solidus, *see* Waxes / Fats, 2915
Adeps solidus W35, *see* Waxes / Fats, 2915
Adrenaline hydrogen tartrate, *see* Epinephrine hydrogen tartrate, 911
Adrenalini tartras, *see* Epinephrine hydrogen tartrate, 911
Aescinum solubile, *see* Escin, water-soluble, 951
Alaninum, *see* L-alanine, 1377
Albendazole, 61
Albendazolum, *see* Albendazole, 61
Alcohol cetylicus, *see* Cetostearyl alcohol, 479
Alcohol cetylicus et stearylicus, *see* Cetostearyl alcohol, 479
Alcohol cetylicus et stearylicus emulsificans A, *see* Cetostearyl alcohol, 479
Alcoholes emulsificantes nonionici, *see* Non-ionic emulsifying alcohol, 1867
Alcoholes lanae, *see* Wool alcohols, 2951
Alfatradiol, 67
Alfatradiolum, *see* Alfatradiol, 67
Allantoin, 79
Allantoinum, *see* Allantoin, 79
Allopurinol, 87
Allopurinolum, *see* Allopurinol, 87
alpha-tocopheryl acetate dry concentrate, 93
alpha-Tocopherylis acetatis pulvis, *see* alpha-tocopheryl acetate dry concentrate, 93
Aluminii chloridum hexahydricum, *see* Aluminium chloride hexahydrate, 99
Aluminium chloride hexahydrate, 99
Ambroxol hydrochloride, 107
Ambroxoli hydrochloridum, *see* Ambroxol hydrochloride, 107
Amifampridine, 119
Amifampridinum, *see* Amifampridine, 119
Amiloride hydrochloride dihydrate, 125
Amiloridi hydrochloridum dihydricum, *see* Amiloride hydrochloride dihydrate, 125
Amitriptyline hydrochloride, 131
Amitriptylini hydrochloridum, *see* Amitriptyline hydrochloride, 131
Amlodipine besilate, 139
Amlodipini besilas, *see* Amlodipine besilate, 139
Ammonii hydrogencarbonas, *see* Ammonium hydrogen carbonate, 143
Ammonium hydrogen carbonate, 143
Amoxicillin trihydrate, 149
Amoxicillinum trihydricum, *see* Amoxicillin trihydrate, 149
Amphotericin B, 155
Amphotericinum B, *see* Amphotericin B, 155
Amylum Maydis, *see* Starch, 2537
Amylum oryzae, *see* Starch, 2537
Argentum proteinicum, *see* Silver protein, 2401
Arginine, 161
Arginine hydrochloride, 167
Arginini hydrochloridum, *see* Arginine hydrochloride, 167
Argininum, *see* Arginine, 161
Ascorbic acid, 173
Ascorbyl palmitate, 181

Ascorbylis palmitas, *see* Ascorbyl palmitate, 181
Aspartic acid, 191
Atropine sulfate, 195
Atropine sulphate, *see* Atropine sulfate, 195
Atropini sulfas, *see* Atropine sulfate, 195

Bacitracin, 201
Bacitracinum, *see* Bacitracin, 201
Baclofen, 209
Baclofenum, *see* Baclofen, 209
Beclometasone dipropionate, 215
Beclometasoni dipropionas, *see* Beclometasone dipropionate, 215
Beeswax, white, *see* Waxes / Fats, 2915
Beeswax, yellow, *see* Waxes / Fats, 2915
Benzocaine, 221
Benzocainum, *see* Benzocaine, 221
Benzoic acid, 231
Benzydamine hydrochloride, 237
Benzydamini hydrochloridum, *see* Benzydamine hydrochloride, 237
Betaine monohydrate, 245
Betainum monohydricum, *see* Betaine monohydrate, 245
Betamethasone, 249
Betamethasone dipropionate, 255
Betamethasone valerate, 269
Betamethasoni dipropionas, *see* Betamethasone dipropionate, 255
Betamethasoni valeras, *see* Betamethasone valerate, 269
Betamethasonum, *see* Betamethasone, 249
Bifonazole, 299
Bifonazolum, *see* Bifonazole, 299
Biotin, 305
Biotinum, *see* Biotin, 305
Bismuth gallath, basic, 311
Bismuthi subgallas, *see* Bismuth gallath, basic, 311
Borax, *see* Sodium tetraborate, 2493
Boric acid, 323
Budesonide, 329
Budesonidum, *see* Budesonide, 329
Bupivacaine hydrochloride, 339
Bupivacaini hydrochloridum, *see* Bupivacaine hydrochloride, 339
Butylated hydroxytoluene, 343
Butylhydroxytoluenum, *see* Butylated hydroxytoluene, 343

Caffeine, 351
Caffeine citrate, 359
Calcii ascorbas dihydricum, *see* Calcium ascorbate dihydrate, 365
Calcii citras tetrahydricus, *see* Calcium citrate tetrahydrate, 371
Calcii gluconas, *see* Calcium gluconate, 379
Calcii glycerophosphas, *see* Calcium glycerophosphate, 387
Calcii hydrogenphosphas dihydricus, *see* Calcium hydrogen phosphate dihydrate, 395
Calcii lactas pentahydricus, *see* Calcium lactate pentahydrate, 401
Calcii pantothenas, *see* Calcium pantothenate, 407
Calcium ascorbate dihydrate, 365
Calcium citrate tetrahydrate, 371
Calcium gluconate, 379
Calcium glycerophosphate, 387
Calcium hydrogen phosphate dihydrate, 395
Calcium lactate pentahydrate, 401
Calcium pantothenate, 407
Camphor, racemic, *see* Camphor, racemic/D-Camphor, 415
Camphor, racemic/D-Camphor, 415
Camphora racemica, *see* Camphor, racemic/D-Camphor, 415
Cannabidiol, 423
Capsacinum, *see* Capsaicin, 437
Capsaicin, 437
Captopril, 443
Captoprilum, *see* Captopril, 443
Carbomera, *see* Carbomers, 453
Carbomers, 453
Carmellose sodium, 465
Carmellosum natricum, *see* Carmellose sodium, 465
Cellulose, microcrystalline, 473
Cellulosum microcristallinum, *see* Cellulose, microcrystalline, 473
Cera alba, *see* Waxes / Fats, 2915
Cera flava, *see* Waxes / Fats, 2915
Cetomacrogol emulsifying wax 1000 NI, *see* Cetostearyl alcohol, 479
Cetostearyl alcohol, 479
Cetyl alcohol, *see* Cetostearyl alcohol, 479
Cetyl palmitate, *see* Waxes / Fats, 2915
Cetylis palmitas, *see* Waxes / Fats, 2915
Chinidini sulfas, *see* Quinidine sulfate dihydrate, 2293
Chinini hydrochloridum dihydricum, *see* Quinine hydrochloride dihydrate, 2299
Chinini sulfas, *see* Quinine sulfate, 2305
Chloral hydrate, 495
Chlorali hydras, *see* Chloral hydrate, 495
Chloramphenicol, 505
Chloramphenicolum, *see* Chloramphenicol, 505
Chlorhexidine diacetate, 523
Chlorhexidini acetas, *see* Chlorhexidine diacetate, 523
Chlorocresol, 533

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Chlorocresolum, *see* Chlorocresol, 533
Chlorprothixene hydrochloride, 539
Chlorprothixeni hydrochloridum, *see* Chlorprothixene hydrochloride, 539
Chlortetracycline hydrochloride, 543
Chlortetracyclini hydrochloridum, *see* Chlortetracycline hydrochloride, 543
Cholesterol, 553
Cholesterolum, *see* Cholesterol, 553
Choline chloride, 561
Choline hydrogen tartrate, 565
Cholinii chloridum, *see* Choline chloride, 561
Cholinium bitartaricum, *see* Choline hydrogen tartrate, 565
Ciclopirox olamine, 571
Ciclopirox olaminum, *see* Ciclopirox olamine, 571
Ciclosporin, 579
Ciclosporinum, *see* Ciclosporin, 579
Ciprofloxacin hydrochloride, 587
Ciprofloxacini hydrochloridum, *see* Ciprofloxacin hydrochloride, 587
Citric acid, 593
Citric acid monohydrate, 617
Citrulline, 625
Citrullinum, *see* Citrulline, 625
Clindamycin hydrochloride, 631
Clindamycin-2-dihydrogen phosphate, 645
Clindamycini hydrochloridum, *see* Clindamycin hydrochloride, 631
Clindamycini phosphas, *see* Clindamycin-2-dihydrogen phosphate, 645
Clioquinol, 651
Clioquinolum, *see* Clioquinol, 651
Clobetasol propionate, 667
Clobetasoli propionas, *see* Clobetasol propionate, 667
Clonidine hydrochloride, 691
Clonidini hydrochloridum, *see* Clonidine hydrochloride, 691
Clotrimazole, 697
Clotrimazolum, *see* Clotrimazole, 697
Cocoa butter, *see* Waxes / Fats, 2915
Coffeini citras, *see* Caffeine citrate, 359
Coffeinum, *see* Caffeine, 351
Colistin sulfate, 731
Colistin sulphate, *see* Colistin sulfate, 731
Colistini sulfas, *see* Colistin sulfate, 731
Corn starch, *see* Starch, 2537
Cromolyn sodium, *see* Sodium cromoglicate, 2451
Cyanocobalamin, *see* Cyanocobalamin / Methylcobalamin, 737
Cyanocobalamin / Methylcobalamin, 737
Cyanocobalaminum, *see* Cyanocobalamin / Methylcobalamin, 737
Cyproheptadine hydrochloride 1.5 hydrate, 743
Cyproheptadini hydrochloridum-1,5-hydricum, *see* Cyproheptadine hydrochloride 1.5 hydrate, 743
Cyproterone acetate, 747
Cyproteroni acetas, *see* Cyproterone acetate, 747
Cysteine hydrochloride monohydrate, 755
Cysteini hydrochloridum monohydricum, *see* Cysteine hydrochloride monohydrate, 755
Cystine, 761
Cystinum, *see* Cystine, 761

D-Camphor, *see* Camphor, racemic/D-Camphor, 415
D-Camphora, *see* Camphor, racemic/D-Camphor, 415
Dequalinii chloridum, *see* Dequalinium chloride, 767
Dequalinium chloride, 767
Dexamethasone, 777
Dexamethasone acetate, 795
Dexamethasoni acetas, *see* Dexamethasone acetate, 795
Dexamethasonum, *see* Dexamethasone, 777
Dextromethorphan hydrobromide monohydrate, 803
Dextromethorphani hydrobromidum monohydricum, *see* Dextromethorphan hydrobromide monohydrate, 803
Diclofenac sodium, 809
Diclofenacum natricum, *see* Diclofenac sodium, 809
Diltiazem hydrochloride, 819
Diltiazemi hydrochloridum, *see* Diltiazem hydrochloride, 819
Dinatrii edetas, *see* Sodium edetate, 2469
Diphenhydramine hydrochloride, 843
Diphenhydramini hydrochloridum, *see* Diphenhydramine hydrochloride, 843
Diphenylcyclopropenone, 849
Diphenylcyclopropenonum, *see* Diphenylcyclopropenone, 849
Dithranol, 855
Dithranolum, *see* Dithranol, 855
DL-Methionine, 865
DL-Methioninum, *see* DL-Methionine, 865
DL-Phenylalanine, *see* L-Phenylalanine, 1441
Doxepin hydrochloride, 869
Doxepini hydrochloridum, *see* Doxepin hydrochloride, 869
Doxycycline hyclate, 875

Doxycyclini hyclas, *see* Doxycycline hyclate, 875
Doxylamine hydrogen succinate, 881
Doxylamine succinate, *see* Doxylamine hydrogen succinate, 881
Doxylamini hydrogenosuccinas, *see* Doxylamine hydrogen succinate, 881

EDTA calcium disodium, 887
Emulsifying cetostearyl alcohol (type A), *see* Cetostearyl alcohol, 479
Enalapril maleate, 893
Enalaprili maleas, *see* Enalapril maleate, 893
Eosin Y, 899
Eosinum natricum, *see* Eosin Y, 899
Ephedrine hydrochloride, 905
Ephedrini hydrochloridum, *see* Ephedrine hydrochloride, 905
Epinephrine hydrogen tartrate, 911
Erythromycin, 917
Erythromycinum, *see* Erythromycin, 917
Escin, water-soluble, 951
Estradiol benzoate, 957
Estradiol hemihydrate, 967
Estradiol valerate, 977
Estradioli benzoas, *see* Estradiol benzoate, 957
Estradioli valeras, *see* Estradiol valerate, 977
Estradiolum hemihydricum, *see* Estradiol hemihydrate, 967
Estriol, 987
Estriolum, *see* Estriol, 987
Ethacridine lactate monohydrate, 997
Ethacridini lactas monohydricus, *see* Ethacridine lactate monohydrate, 997
Ethinylestradiol, 1005
Ethinylestradiolum, *see* Ethinylestradiol, 1005
Ethosuximide, 1011
Ethosuximidum, *see* Ethosuximide, 1011

Fampridine, 1015
Fampridinum, *see* Fampridine, 1015
Ferrosi gluconas hydricus, *see* Ferrous gluconate hydrate, 1021
Ferrous gluconate hydrate, 1021
Finasteride, 1025
Finasteridum, *see* Finasteride, 1025
Fluocinolone acetonide, 1031
Fluocinoloni acetonidum, *see* Fluocinolone acetonide, 1031
Folic acid hydrate, 1037
Fructose, 1043
Fructosum, *see* Fructose, 1043
Furosemide, 1057
Furosemidum, *see* Furosemide, 1057
Fusidic acid, 1063

Gabapentin, 1069
Gabapentinum, *see* Gabapentin, 1069
Galactose, 1073
Galactosum, *see* Galactose, 1073
Gelatina alba, *see* Gelatine, white, 1079
Gelatine, white, 1079
Gentamicin sulfate, 1085
Gentamicin sulphate, *see* Gentamicin sulfate, 1085
Gentamicini sulfas, *see* Gentamicin sulfate, 1085
Glucose, 1103
Glucose monohydrate, 1115
Glucosum, *see* Glucose, 1103
Glucosum monohydricum, *see* Glucose monohydrate, 1115
Glutamic acid, 1137
Glutamine, 1143
Glutaminum, *see* Glutamine, 1143
Glutathione, 1149
Glutathionum, *see* Glutathione, 1149
Glycerol monostearate 40-55, *see* Monostereates, 1779
Glycerol monostearate 60, *see* Monostereates, 1779
Glycerol monostearate, emulsifying, *see* Monostereates, 1779
Glyceroli monostearas 40–55, *see* Monostereates, 1779
Glyceroli monostearates 60, *see* Monostereates, 1779
Glyceroli monostearates emulsificantes, *see* Monostereates, 1779
Glycine, 1155
Glycinum, *see* Glycine, 1155
Glycopyrronii bromidum, *see* Glycopyrronium bromide, 1161
Glycopyrronium bromide, 1161
Gramicidin, 1167
Gramicidinum, *see* Gramicidin, 1167
Griseofulvin, 1173
Griseofulvinum, *see* Griseofulvin, 1173
Guaifenesin, 1179
Guaifenesinum, *see* Guaifenesin, 1179

Hard fat, *see* Waxes / Fats, 2915
Hard fat W35, *see* Waxes / Fats, 2915
Heparin sodium, 1185
Heparinum natricum, *see* Heparin sodium, 1185
Histamine dihydrochloride, 1191
Histamini dihydrochloridum, *see* Histamine dihydrochloride, 1191
Histidine, 1197
Histidinum, *see* Histidine, 1197
Homatropine hydrobromide, 1203

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Homatropini hydrobromidum, *see* Homatropine hydrobromide, 1203
Hydrochinonum, *see* Hydroquinone, 1265
Hydrochlorothiazide, 1207
Hydrochlorothiazidum, *see* Hydrochlorothiazide, 1207
Hydrocortisone, 1215
Hydrocortisone acetate, 1239
Hydrocortisoni acetas, *see* Hydrocortisone acetate, 1239
Hydrocortisonum, *see* Hydrocortisone, 1215
Hydroquinone, 1265
Hydroxyethyl cellulose, 1273
Hydroxyethylcellulosum, *see* Hydroxyethyl cellulose, 1273
Hydroxypropylcellulose, *see* Methylcellulose, 1659
Hydroxypropylcellulosum, *see* Methylcellulose, 1659
Hyoscine butylbromide, 1279
Hyoscine hydrobromide, 1285
Hyoscini butylbromidum, *see* Hyoscine butylbromide, 1279
Hypromellose, *see* Methylcellulose, 1659
Hypromellosum, *see* Methylcellulose, 1659

Ibuprofen, 1293
Ibuprofenum, *see* Ibuprofen, 1293
Indometacin, 1299
Indometacinum, *see* Indometacin, 1299
Iodoform, 1305
Iodoformium, *see* Iodoform, 1305
Ipratropii bromidum, *see* Ipratropium bromide, 1315
Ipratropium bromide, 1315
Isoleucine, 1321
Isoleucinum, *see* Isoleucine, 1321
Isorbidi dinitras 40%, *see* Isosorbide dinitrate 40%, 1327
Isosorbide dinitrate 40%, 1327
Isoxsuprine hydrochloride, 1339
Isoxsuprini hydrochloridum, *see* Isoxsuprine hydrochloride, 1339
Ivermectin, 1343
Ivermectinum, *see* Ivermectin, 1343

Kalii citras, *see* Potassium citrate, 2053
Kalii dihydrogenophosphas, *see* potassium dihydrogen phosphate, 2063
Kalii hydrogencarbonas, *see* Potassium hydrocarbonate, 2067
Kalii hydrogentartras, *see* Potassium hydrogen tartrate, 2073
Kalii sorbas, *see* Potassium sorbate, 2079
Ketamine hydrochloride, 1347
Ketamini hydrochloridum, *see* Ketamine hydrochloride, 1347
Ketoconazole, 1353
Ketoconazolum, *see* Ketoconazole, 1353

L-alanine, 1377
L-citrulline, *see* Citrulline, 625
L-glutamine, *see* Glutamine, 1143
L-histidine, *see* Histidine, 1197
L-isoleucine, *see* Isoleucine, 1321
L-Phenylalanine, 1441
L-serine, *see* Serine, 2385
L-Threonine, 1447
Lactose monohydrate, 1359
Lactosum monohydricum, *see* Lactose monohydrate, 1359
Lecithinum e sojae plv., *see* Soy lecithin (instant form), 2519
Leucine, 1381
Leucinum, *see* Leucine, 1381
Levocarnitine, 1387
Levocarnitinum, *see* Levocarnitine, 1387
Levothyroxin sodium, 1393
Levothyroxinum natrii, *see* Levothyroxin sodium, 1393
Lidocaine, 1399
Lidocaine hydrochloride monohydrate, 1415
Lidocaini hydrochloridum monohydricum, *see* Lidocaine hydrochloride monohydrate, 1415
Lidocainum, *see* Lidocaine, 1399
Lithii orotas monohydricum, *see* Lithium orotate monohydrate, 1435
Lithium orotate monohydrate, 1435
Lysine HCl, *see* Lysine hydrochloride, 1453
Lysine hydrochloride, 1453
Lysini hydrochloridum, *see* Lysine hydrochloride, 1453

Macrogols 1500, 1459
Macrogols 4000, 1465
Macrogolum 1500, *see* Macrogols 1500, 1459
Macrogolum 4000, *see* Macrogols 4000, 1465
Mafenide acetate, 1485
Mafenidum aceticum, *see* Mafenide acetate, 1485
Magnesii aspartas tetrahydricus, *see* Magnesium hydrogen aspartate tetrahydrate, 1501
Magnesii chloridum hexahydricum, *see* Magnesium chloride hexahydrate, 1489
Magnesii citras, *see* Magnesium citrate, 1495
Magnesii hydrogenocitras hydricus, *see* Magnesium hydrogen citrate, 1507
Magnesii orotas dihydricus, *see* Magnesium orotate dihydrate, 1519
Magnesii stearas, *see* Magnesium stearate, 1525

Magnesii sulfas heptahydricus, *see* Magnesium sulfate heptahydrate, 1531
Magnesium chloride hexahydrate, 1489
Magnesium citrate, 1495
Magnesium hydrogen aspartate tetrahydrate, 1501
Magnesium hydrogen citrate, 1507
Magnesium hydrogen citrate, hydrated, *see* Magnesium hydrogen citrate, 1507
Magnesium orotate dihydrate, 1519
Magnesium stearate, 1525
Magnesium sulfate heptahydrate, 1531
Magnesium sulphate heptahydrate, *see* Magnesium sulfate heptahydrate, 1531
Maltodextrin, 1537
Maltodextrinum, *see* Maltodextrin, 1537
Manganese orotate dihydrate, 1543
Manganese sulfate monohydrate, 1549
Manganese sulphate monohydrate, *see* Manganese sulfate monohydrate, 1549
Mangani sulfas monohydricus, *see* Manganese sulfate monohydrate, 1549
Mannitol, 1553
Mannitolum, *see* Mannitol, 1553
Melatonin, 1579
Melatoninum, *see* Melatonin, 1579
Menthol, 1593
Mentholum, *see* Menthol, 1593
Mepivacaine hydrochloride, 1611
Mepivacaini hydrochloridum, *see* Mepivacaine hydrochloride, 1611
Mesalazine, 1617
Mesalazinum, *see* Mesalazine, 1617
Metamizol sodium monohydrate, 1623
Metamizolum natricum monohydricum, *see* Metamizol sodium monohydrate, 1623
Methacholine chloride, 1629
Methacholinii chloridum, *see* Methacholine chloride, 1629
Methionine, 1635
Methioninum, *see* Methionine, 1635
Methoxsalen, 1641
Methoxsalenum, *see* Methoxsalen, 1641
Methyl-4-hydroxybenzoate, 1651
Methylcellulose, 1659
Methylcellulosum, *see* Methylcellulose, 1659
Methylcobalamin, *see* Cyanocobalamin / Methylcobalamin, 737
Methylis parahydroxybenzoas, *see* Methyl-4-hydroxybenzoate, 1651
Methylprednisolone, 1671
Methylprednisolonum, *see* Methylprednisolone, 1671
Metoclopramide hydrochloride monohydrate, 1677
Metoclopramidi hydrochloridum monohydricum, *see* Metoclopramide hydrochloride monohydrate, 1677
Metoprolol tartrate, 1683
Metoprololi tartras, *see* Metoprolol tartrate, 1683
Metronidazole, 1689
Metronidazolum, *see* Metronidazole, 1689
Miconazole nitrate, 1717
Miconazoli nitras, *see* Miconazole nitrate, 1717
Microcrystalline wax, *see* Waxes / Fats, 2915
Minoxidil, 1737
Minoxidilum, *see* Minoxidil, 1737
Mometasone furoate, 1759
Mometasoni furoas, *see* Mometasone furoate, 1759
Monostereates, 1779
Mupirocin calcium, 1789
Mupirocinum calcicum, *see* Mupirocin calcium, 1789
myo-Inositol, 1795
myo-Inositolum, *see* myo-Inositol, 1795

Naloxone hydrochloride dihydrate, 1799
Naloxoni hydrochloridum dihydricum, *see* Naloxone hydrochloride dihydrate, 1799
Naltrexone hydrochloride, 1805
Naltrexoni hydrochloridum, *see* Naltrexone hydrochloride, 1805
Naphazoline hydrochloride, 1809
Naphazoline nitrate, 1817
Naphazolini hydrochloridum, *see* Naphazoline hydrochloride, 1809
Naphazolini nitras, *see* Naphazoline nitrate, 1817
Naproxen, 1823
Naproxenum, *see* Naproxen, 1823
Natrii acetas trihydricum, *see* Sodium acetate trihydrate, 2407
Natrii ascorbas, *see* Sodium ascorbate, 2413
Natrii benzoas, *see* Sodium benzoate, 2419
Natrii calcii edetas, *see* EDTA calcium disodium, 887
Natrii citras, *see* Sodium citrate, 2433
Natrii cromoglicas, *see* Sodium cromoglicate, 2451
Natrii cyclamas, *see* Sodium cyclamate, 2457
Natrii dihydrogenophosphas dihydricus, *see* Sodium dihydrogen phosphate dihydrate, 2463
Natrii laurilsulfas, *see* Waxes / Fats, 2915
Natrii salicylas, *see* Sodium salicylate, 2481

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Natrii sulfas decahydricus, *see* Sodium sulfate decahydrate, 2487
Neomycin sulfate, 1827
Neomycin sulphate, *see* Neomycin sulfate, 1827
Neomycini sulfas, *see* Neomycin sulfate, 1827
Neostigmine bromide, 1839
Neostigmini bromidum, *see* Neostigmine bromide, 1839
Nicotinamide, 1845
Nicotinamidum, *see* Nicotinamide, 1845
Nicotinic acid, 1851
Nifedipine, 1857
Nifedipinum, *see* Nifedipine, 1857
Nitrofurantoin, 1861
Nitrofurantoinum, *see* Nitrofurantoin, 1861
Non-ionic emulsifying alcohol, 1867
Norethisterone acetate, 1873
Norethisteroni acetas, *see* Norethisterone acetate, 1873
Noscapine hydrochloride hydrate, 1879
Noscapini hydrochloridum hydricum, *see* Noscapine hydrochloride hydrate, 1879
Nystatin, 1883
Nystatinum, *see* Nystatin, 1883

Octenidine dihydrochloride, 1899
Octenidini dihydrochloridum, *see* Octenidine dihydrochloride, 1899
Ofloxacin, 1913
Ofloxacinum, *see* Ofloxacin, 1913
Omeprazole, 1919
Omeprazolum, *see* Omeprazole, 1919
Ornithine aspartate, 1927
Ornithine hydrochloride, 1933
Ornithini aspartas, *see* Ornithine aspartate, 1927
Ornithini hydrochloridum, *see* Ornithine hydrochloride, 1933
Oxalic acid, 1939
Oxetacaine, 1945
Oxetacainum, *see* Oxetacaine, 1945
Oxybuprocaine hydrochloride, 1951
Oxybuprocaini hydrochloridum, *see* Oxybuprocaine hydrochloride, 1951
Oxybutynin hydrochloride, 1957
Oxybutynini hydrochloridum, *see* Oxybutynin hydrochloride, 1957
Oxytetracycline hydrochloride, 1965
Oxytetracyclini hydrochloridum, *see* Oxytetracycline hydrochloride, 1965

Pancreas powder, 1975
Pancreatis pulvis, *see* Pancreas powder, 1975
Papaverine hydrochloride, 1979
Papaverini hydrochloridum, *see* Papaverine hydrochloride, 1979
Paracetamol, 1985
Paracetamolum, *see* Paracetamol, 1985
Paraffin, hard, *see* Waxes / Fats, 2915
Paraffin, microcrystalline, *see* Waxes / Fats, 2915
Paraffina microcristallina, *see* Waxes / Fats, 2915
Paraffinum solidum, *see* Waxes / Fats, 2915
Patent blue V, 1993
Pectin, 1999
Phenazone, 2003
Phenazonum, *see* Phenazone, 2003
Pheniramine maleate, 2009
Pheniramini maleas, *see* Pheniramine maleate, 2009
Phenylalanine, *see* L-Phenylalanine, 1441
Phenylalaninum, *see* L-Phenylalanine, 1441
Phenylbutazon, 2015
Phenylbutazonum, *see* Phenylbutazon, 2015
Phenylephrine hydrochloride, 2021
Phenylephrini hydrochloridum, *see* Phenylephrine hydrochloride, 2021
Phenytoin, 2027
Phenytoinum, *see* Phenytoin, 2027
Pilocarpine hydrochloride, 2033
Pilocarpini hydrochloridum, *see* Pilocarpine hydrochloride, 2033
Poloxamera, *see* Poloxamers, 2039
Poloxamers, 2039
Polymyxin B sulfate, 2045
Polymyxin B sulphate, *see* Polymyxin B sulfate, 2045
Polymyxini B sulfas, *see* Polymyxin B sulfate, 2045
Potassium citrate, 2053
potassium dihydrogen phosphate, 2063
Potassium guaiacolsulfonate, *see* Sulfogaiacol hydrate, 2593
Potassium hydrocarbonate, 2067
Potassium hydrogen tartrate, 2073
Potassium sorbate, 2079
Potato starch, *see* Starch, 2537
Povidone, 2093
Povidone iodine, 2101
Povidonum, *see* Povidone, 2093
Povidonum iodinatum, *see* Povidone iodine, 2101
Prasterone, 2109
Prasteronum, *see* Prasterone, 2109
Praziquantel, 2117
Praziquantelum, *see* Praziquantel, 2117
Prednicarbate, 2121
Prednicarbatum, *see* Prednicarbate, 2121
Prednisolon dihydrogen phosphate dinatrium, 2143
Prednisolone, 2151
Prednisolone acetate, 2171

Prednisolone hydrogen succinate, 2191
Prednisoloni acetas, *see* Prednisolone acetate, 2171
Prednisoloni hydrogenosuccinas, *see* Prednisolone hydrogen succinate, 2191
Prednisoloni natrii phosphas, *see* Prednisolon dihydrogen phosphate dinatrium, 2143
Prednisolonum, *see* Prednisolone, 2151
Prednisone, 2197
Prednisonum, *see* Prednisone, 2197
Pregnenolone, 2203
Pregnenolonum, *see* Pregnenolone, 2203
Prilocaine, 2209
Prilocaine hydrochloride, 2213
Prilocaini hydrochloridum, *see* Prilocaine hydrochloride, 2213
Prilocainum, *see* Prilocaine, 2209
Procaine hydrochloride, 2219
Procaini hydrochloridum, *see* Procaine hydrochloride, 2219
Progesterone, 2227
Progesteronum, *see* Progesterone, 2227
Proline, 2247
Prolinum, *see* Proline, 2247
Propranolol hydrochloride, 2253
Propranololi hydrochloridum, *see* Propranolol hydrochloride, 2253
Propyl-4-hydroxybenzoate, 2265
Propylis parahydroxybenzoas, *see* Propyl-4-hydroxybenzoate, 2265
Propyphenazone, 2271
Propyphenazonum, *see* Propyphenazone, 2271
Pyridoxal-5-phosphate, 2277
Pyridoxali phosphas, *see* Pyridoxal-5-phosphate, 2277
Pyridoxine hydrochloride, 2283
Pyridoxini hydrochloridum, *see* Pyridoxine hydrochloride, 2283

Quetiapine fumarate, 2289
Quetiapini fumaras, *see* Quetiapine fumarate, 2289
Quinidine sulfate, *see* Quinidine sulfate dihydrate, 2293
Quinidine sulfate dihydrate, 2293
Quinine hydrochloride dihydrate, 2299
Quinine sulfate, 2305
Quinoline yellow, 2311

Resocrinol, 2317
Resorcinolum, *see* Resocrinol, 2317
Riboflavin, 2325
Riboflavin sodium phosphate hydrate, 2333
Riboflavini natrii phosphas hydricum, *see* Riboflavin sodium phosphate hydrate, 2333
Riboflavinum, *see* Riboflavin, 2325
Rice starch, *see* Starch, 2537
Ropivacaine hydrochloride monohydrate, 2339
Ropivacaini hydrochloridum monohydricum, *see* Ropivacaine hydrochloride monohydrate, 2339

Saccharin sodium, 2343
Saccharinum natricum, *see* Saccharin sodium, 2343
Saccharum, *see* Sucrose, 2561
Salbutamol sulfate, 2351
Salbutamol sulphate, *see* Salbutamol sulfate, 2351
Salbutamoli sulfas, *see* Salbutamol sulfate, 2351
Salicylic acid, 2355
Scopolamini hydrobromidum, *see* Hyoscine hydrobromide, 1285
Selenium yeast, 2379
Serine, 2385
Serinum, *see* Serine, 2385
Sildenafil citrate, 2391
Sildenafili citras, *see* Sildenafil citrate, 2391
Silver protein, 2401
Sodium acetate trihydrate, 2407
Sodium ascorbate, 2413
Sodium benzoate, 2419
Sodium calcium edetate, *see* EDTA calcium disodium, 887
Sodium chondroitin sulfate, 2429
Sodium chondroitin sulphate, *see* Sodium chondroitin sulfate, 2429
Sodium citrate, 2433
Sodium cromoglicate, 2451
Sodium cyclamate, 2457
Sodium dihydrogen phosphate dihydrate, 2463
Sodium dodecyl sulfate, *see* Waxes / Fats, 2915
Sodium dodecyl sulphate, *see* Waxes / Fats, 2915
Sodium edetate, 2469
Sodium saccharin, *see* Saccharin sodium, 2343
Sodium salicylate, 2481
Sodium sulfate decahydrate, 2487
Sodium sulphate decahydrate, *see* Sodium sulfate decahydrate, 2487
Sodium tetraborate, 2493
Solani amylum, *see* Starch, 2537
Sorbic acid, 2499
Sorbitan stearate, *see* Monostereates, 1779
Sorbitani stearas, *see* Monostereates, 1779
Sorbitol, 2507
Sorbitolum, *see* Sorbitol, 2507
Sotalol hydrochloride, 2515

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*

Sotaloli hydrochloridum, *see* Sotalol hydrochloride, 2515
Soy lecithin (instant form), 2519
Spironolactone, 2525
Spironolactonum, *see* Spironolactone, 2525
Starch, 2537
Stearic acid 50, 2555
Sucrose, 2561
Sulfacetamide, 2581
Sulfacetamidum, *see* Sulfacetamide, 2581
Sulfadiazine, 2587
Sulfadiazinum, *see* Sulfadiazine, 2587
Sulfogaiacol hydrate, 2593
Sulfoguaiacolum hydricum, *see* Sulfogaiacol hydrate, 2593
Sulpiride, 2599
Sulpiridum, *see* Sulpiride, 2599
SyrSpend® SF Alka, *see* Starch, 2537
SyrSpend® SF pH4, *see* Starch, 2537
SyrSpend® SF pH4 neo (Maize starch), *see* Starch, 2537

Tacrolimus monohydrate , 2603
Tacrolimusum monohydricum, *see* Tacrolimus monohydrate , 2603
Tannin, 2609
Tanninum, *see* Tannin, 2609
Tartaric acid, 2619
Taurine, 2629
Taurinum, *see* Taurine, 2629
Testosterone, 2635
Testosterone propionate, 2643
Testosteroni propionas, *see* Testosterone propionate, 2643
Testosteronum, *see* Testosterone, 2635
Tetracaine, 2655
Tetracaine hydrochloride, 2665
Tetracaini hydrochloridum, *see* Tetracaine hydrochloride, 2665
Tetracainum, *see* Tetracaine, 2655
Tetracycline hydrochloride, 2681
Tetracyclini hydrochloridum, *see* Tetracycline hydrochloride, 2681
Theobromatis oleum, *see* Waxes / Fats, 2915
Theophylline, 2691
Theophylline-ethylenediamine hydrate, 2697
Theophyllinum, *see* Theophylline, 2691
Theophyllinum et ethylendiaminum hydricum, *see* Theophylline-ethylenediamine hydrate, 2697
Thiamine chloride hydrochloride, 2703
Thiamini hydrochloridum, *see* Thiamine chloride hydrochloride, 2703
Thiomersal, 2709
Thiomersalum, *see* Thiomersal, 2709
Threonine, *see* L-Threonine, 1447
Threoninum, *see* L-Threonine, 1447
Thymol, 2715
Thymolum, *see* Thymol, 2715
Tobramycin sulfate, 2723
Tobramycin sulphate, *see* Tobramycin sulfate, 2723
Tobramycini sulfas, *see* Tobramycin sulfate, 2723
Tosylchloramide sodium, 2729
Tosylchloramidum natricum, *see* Tosylchloramide sodium, 2729
Tranexamic acid, 2735
Tretinoin, 2741
Tretinoinum, *see* Tretinoin, 2741
Triamcinolone, 2757
Triamcinolone acetonide, 2763
Triamcinoloni acetonidum, *see* Triamcinolone acetonide, 2763
Triamcinolonum, *see* Triamcinolone, 2757
Triclosan, 2793
Triclosanum, *see* Triclosan, 2793
Tritici amylum, *see* Starch, 2537
Trometamol, 2823
Trometamolum, *see* Trometamol, 2823
Tropicamide, 2835
Tropicamidum, *see* Tropicamide, 2835
Tryptophan, 2841
Tryptophanum, *see* Tryptophan, 2841
Tyrosine, 2847
Tyrosinum, *see* Tyrosine, 2847
Tyrothricin, 2853
Tyrothricinum, *see* Tyrothricin, 2853

Ubidecarenone, 2859
Ubidecarenonum, *see* Ubidecarenone, 2859
Urea, 2865
Ureum, *see* Urea, 2865
Ursodeoxycholic acid, 2893

Valine, 2897
Valinum, *see* Valine, 2897
Vancomycin hydrochloride, 2903
Vancomycini hydrochloridum, *see* Vancomycin hydrochloride, 2903
Vanillin, 2909
Vanillinum, *see* Vanillin, 2909

Waxes / Fats, 2915
Wheat starch, *see* Starch, 2537
Wool alcohols, 2951

Xylitol, 2957
Xylitolum, *see* Xylitol, 2957
Xylometazoline hydrochloride, 2963
Xylometazolini hydrochloridum, *see* Xylometazoline hydrochloride, 2963
Xylose, 2971
Xylosum, *see* Xylose, 2971

Zinc acetate dihydrate, 2977
Zinc gluconate, 2983
Zinc orotate dihydrate, 2989
Zinc stearate, 2993
Zinc sulfate heptahydrate, 2997
Zinc sulphate heptahydrate, *see* Zinc sulfate heptahydrate, 2997
Zinci acetas dihydricus, *see* Zinc acetate dihydrate, 2977
Zinci gluconas, *see* Zinc gluconate, 2983
Zinci stearas, *see* Zinc stearate, 2993
Zinci sulfas heptahydricus, *see* Zinc sulfate heptahydrate, 2997
Zincum oroticum dihydricum, *see* Zinc orotate dihydrate, 2989

© HiperScan GmbH, *ValidationTool 2.9.0* and *ReportingTool 2.9.2*, Report *50-2.9-2025-01*